A new analytic approach to physical observables in QCD

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Dedicated to my Mother:

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Abstract

An analytic ghost-free model for the QCD running coupling $\alpha(Q^2)$ is proposed. It is constructed from a more general approach we developed particularly for investigating physical observables of the type $F(Q^2)$ in regions that are inaccessible to perturbative methods of quantum field theory. This approach directly links the infrared (IR) and the ultraviolet(UV) regions together under the causal analyticity requirement in the complex Q^2-plane. Due to the inclusion of crucial non-perturbative effects, the running coupling in our model not only excludes unphysical singularities but also freezes to a finite value at the IR limit $Q^2 = 0$. This makes it consistent with a popular phenomenological hypothesis, namely the IR freezing phenomenon. Applying this model to compute the Gluon condensate, we obtain a result that is in good agreement with the most recent phenomenological estimate. Having calculated the $\beta-$function corresponding to our QCD coupling constant, we find that it behaves qualitatively like its perturbative counterpart, when calculated beyond the leading order and with a number of quark flavours allowing for the occurrence of IR fixed points.

A further application of our analytic approach in the area of wave functionals has been included. We have proven the existence of a local expansion for the logarithm of the Schrödinger vacuum functional in any scalar field theory with a non-zero mass gap. This expansion is expected to converge for source fields $\varphi(x)$ whose Fourier transforms $\widetilde{\varphi}(k)$ have sufficiently small supports. We have demonstrated how to reconstruct the vacuum functional for an arbitrary source $\varphi(x)$ from the local expansion of its logarithm by exploiting analyticity in a complex scale parameter.

Declaration

The work presented in this thesis is based on research carried out by the author under the supervision of Professor Paul Mansfield at the Centre of Particle Theory, Department of Mathematical Sciences, University of Durham, England.

No part of this thesis has been submitted elsewhere for any other degree or qualification and it is all my own work apart from some introductory materials in chapter 1, 4 and 5.

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Contents

List of Figures

List of Tables

Chapter 1

Introduction

1.1 QCD as a gauge theory

Local gauge symmetries play a central role in the modern theory of particle physics. They provide a useful theoretical paradigm by which a deep insight into the nature of particle interactions can be gained. When constructing a locally gauge-invariant theory we are forced to introduce new fields, referred to as gauge fields, to achieve the required gauge symmetry. From this viewpoint, local gauge invariance restricts the form of the Lagrangian of the theory under the gauge consideration, determining the interaction terms uniquely.

Quantum electrodynamics (QED) is the simplest example of a gauge theory of a physical system and serves as a prototype for quantum chromodynamics (QCD) [1, 2]. It is, therefore, instructive to begin this section with a short review of the derivation of the QED Lagrangian by imposing the requirement of local gauge invariance [2] on Dirac free electron theory, showing how this condition introduces a new vector field $A_\mu(x)$, called the gauge boson field, which identifies the photon. Then, we go on to extend this argument to include QCD.

Consider the famous Dirac Lagrangian for a free spin-1/2 particle of mass m [3]:

$$\mathcal{L} = \overline{\psi}(x)(i\gamma^\mu \partial_\mu - m)\psi(x)\,, \tag{1.1}$$

where $\psi(x)$ is a 4-component fermionic field, called Dirac spinor, $\overline{\psi}(x) = \psi^\dagger(x)\gamma^0$ is the adjoint spinor to $\psi(x)$ and γ^μ denotes the 4×4 Dirac matrices satisfying the anticommutation

relations:

$$\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}\,, \tag{1.2}$$

where $g^{\mu\nu}$ is the Minkowski metric tensor:

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{1.3}$$

Now, under the so-called gauge transformations[1]:

$$\psi(x) \to \psi'(x) = \mathrm{e}^{i\theta}\,\psi(x) \qquad \text{and} \qquad \overline{\psi}(x) \to \overline{\psi'}(x) = \mathrm{e}^{-i\theta}\,\overline{\psi}(x)\,, \tag{1.4}$$

we find that if we fix the arbitrary gauge angle θ such that $\partial_\mu\theta = 0$ the form of the Lagrangian in (1.1) remains unchanged, in which case we have a globally invariant theory. On the other hand, if we allow θ to be space-time dependent, in which case (1.4) is called local gauge transformations, we do not achieve the desired gauge invariance as the Lagrangian in this case transforms according to:

$$\mathcal{L} \to \mathcal{L}' = \mathcal{L} - \overline{\psi}(x)\,\gamma^\mu\,\psi(x)\,\partial_\mu\theta(x)\,. \tag{1.5}$$

This shows how the non-vanishing derivative $\partial_\mu\theta$ spoils the local gauge symmetry of $\mathcal{L}$ and causes the theory to be phase dependent everywhere in Minkowski space-time, which is physically unacceptable.

Now, if we require the Lagrangian $\mathcal{L}$ to remain invariant under local gauge transformations we must modify it by replacing the gradient ∂_μ in its formulation with a covariant derivative D_μ, which transforms under local gauge transformations like the field ψ itself:

$$D_\mu\psi(x) \to [D_\mu\psi(x)]' \equiv D'_\mu\psi'(x) = \mathrm{e}^{i\theta(x)}\,D_\mu\psi(x)\,. \tag{1.6}$$

To construct this covariant derivative, we are forced to introduce a new vector field $A_\mu(x)$ into the definition of D_μ, giving:

$$D_\mu = \partial_\mu + i\,e\,A_\mu(x)\,, \tag{1.7}$$

[1] If the name "gauge transformations" has not been used for historical reasons, these transformations would probably have been called "phase transformations".

such that $A_\mu(x)$ transforms simultaneously with ψ according to:

$$A_\mu \to A'_\mu = A_\mu - \frac{1}{e}\,\partial_\mu\theta\,. \tag{1.8}$$

Here, e is a free parameter which we shall eventually identify as the electric charge of the Dirac field. To check (1.6), we simply transform $D_\mu\psi(x)$ according to (1.4) and (1.8) concurrently, yielding:

$$\begin{aligned} D_\mu\psi \to D'_\mu\psi' &= (\partial_\mu + i\,e\,A'_\mu)\,\mathrm{e}^{i\theta}\,\psi = [\,\partial_\mu + i\,e\,(A_\mu - \frac{1}{e}\,\partial_\mu\theta)\,]\,\mathrm{e}^{i\theta}\,\psi \\ &= \mathrm{e}^{i\theta}\,(\partial_\mu + i\,e\,A_\mu)\,\psi = \mathrm{e}^{i\theta}\,D_\mu\psi\,. \end{aligned} \tag{1.9}$$

This ensures that the new modified Lagrangian:

$$\mathcal{L} = \overline{\psi}\,(i\gamma^\mu D_\mu - m)\,\psi = \overline{\psi}\,(i\gamma^\mu\partial_\mu - m)\,\psi - e\,\overline{\psi}\gamma^\mu\psi\,A_\mu\,, \tag{1.10}$$

is locally invariant under the simultaneous gauge transformations (1.4) and (1.8). The last term in (1.10) corresponds to the interaction between the gauge field $A_\mu(x)$ and the fermionic field $\psi(x)$, showing how they are coupled with strength e. The unique determination of this term is entirely due to the requirement of local gauge symmetry.

To complete the physical construction of a locally invariant Lagrangian, we must add a kinetic energy term for the gauge field $A_\mu(x)$ as it is to represent the photon field. This term can only depend on $A_\mu(x)$ and its derivatives, but not on $\psi(x)$, in such a way that leaves it invariant under the gauge transformation (1.8). Since the familiar electromagnetic field tensor:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu\,, \tag{1.11}$$

is invariant under (1.8), any function that depends on $A_\mu(x)$ only through $F_{\mu\nu}$ and its derivatives is also invariant under (1.8). In classical electrodynamics, the gauge field A_ν and its derivative $\partial_\mu A_\nu$ can be thought of as a generalized coordinate and generalized velocity [4], respectively. Hence, in analogy with the situation with discrete particles we expect the missing Kinetic energy term $\mathcal{L}_{K.E}$ to be quadratic in the velocities, i.e. in $\partial_\mu A_\nu$ or $F_{\mu\nu}$. In addition, $\mathcal{L}_{K.E}$ must be a Lorentz scalar in order to preserve the Lorentz-invariant nature of the action, i.e. $\int \mathcal{L}_{K.E}\,d^4x$. Since the only Lorentz-invariant quadratic

forms which are also invariant under (1.8) are of the type $F_{\mu\nu}F^{\mu\nu}$ [4], it is appropriate enough, with this motivation, to take:

$$\mathcal{L}_{K.E} = -\frac{1}{4} F_{\mu\nu}F^{\mu\nu} . \tag{1.12}$$

Here, the factor of -1/4 is conventional. Note that (1.12) is actually the free Maxwell Lagrangian as one might have guessed [4]. Neglecting gauge fixing terms, we can now write the Lagrangian of QED as:

$$\mathcal{L}_{QED} = \overline{\psi}\,(i\gamma^{\mu}\partial_{\mu} - m)\,\psi - e\,\overline{\psi}\gamma^{\mu}\psi\,A_{\mu} - \frac{1}{4} F_{\mu\nu}F^{\mu\nu} . \tag{1.13}$$

This is a locally gauge-invariant Lagrangian, describing a field theory in which an electron of mass m and charge e is interacting with a massless photon. Note that the addition of a mass term $m_p^2\, A_{\mu}A^{\mu}$ to $\mathcal{L}_{QED}$ is prohibited by the principle of gauge invariance, indicating that the gauge particle, i.e. the photon, is massless.

In summary, we have seen that by imposing the requirement of local gauge symmetry on the free Dirac Lagrangian, we are led to the interacting field theory of QED. The success of this approach motivates us to use it again for deriving the Lagrangian of QCD. But before we do this, let us consider the nature of the gauge transformation in (1.4). The family of phase transformations $U(\theta) = \mathrm{e}^{i\theta}$, depending on one parameter θ as in (1.4), form an Abelian group of unitary 1×1 matrices known as the $U(1)$ group. By an Abelian group we mean that all of the elements in the group commute with each other under the group multiplication, i.e. $U(\theta)U(\theta') = U(\theta')U(\theta)$. In general, any field theory associated with a noncommutative group of phase transformations is termed a *non*-Abelian gauge theory otherwise it is called Abelian gauge theory, just like QED.

QCD is a *non*-Abelian gauge theory, describing the strong colour interactions of quarks, spin-1/2 particles, through the exchange of an octet of massless, spin-1 and colour[2] carrying vector gauge bosons,called gluons. Unlike QED, the symmetry to be gauged in QCD is a *non*-Abelian $SU(3)$ gauge symmetry based on the colour degree of freedom carried by the quarks and gluons. The colour charge hypothesis in QCD was originally proposed to

[2]the term"*colour*" in QCD has absolutely no connection with the ordinary meaning of the word. It is simply used to denote three new quantum numbers.

resolve the problem of the apparent violation of the Pauli exclusion principle by the baryons such as $\Delta^{++}(uuu)$ and $\Omega^{-}(sss)$, which appeared to accommodate three identical quarks in the same state. According to this hypothesis any quark of the six known flavours (i.e. species) must carry a unit of any of the three colour charges: Red, Green and Blue usually denoted by R, G and B respectively. In other words, each quark flavour is supposed to come in three and only three colours, forming a fundamental colour triplet representation of an $SU(3)$ group of phase transformations under which the QCD Lagrangian admits local invariance.

Before going any further, let us now briefly review the properties of the $SU(3)$ group, *the special unitary group in 3 dimensions* [3]. The group $SU(3)$ consists of all unitary 3×3 matrices with unit determinants, i.e. any 3×3 matrix which satisfies the conditions:

$$\mathbf{U}^{\dagger}\mathbf{U} = \mathbf{U}\mathbf{U}^{\dagger} = \mathbf{I} \qquad \text{and} \qquad \det \mathbf{U} = 1\,, \tag{1.14}$$

is an element of the $SU(3)$ group. Phase transformation matrices of the type[4]:

$$\mathbf{U} = \mathrm{e}^{i\mathbf{H}}\,, \tag{1.15}$$

where $\mathbf{H}$ is a 3×3 matrix, form a good representation of the $SU(3)$ group provided that $\mathbf{H}$ is both traceless and Hermitian. The requirement of Hermiticity and tracelessness of $\mathbf{H}$ can be checked from (1.14) with ease. For example, from $\mathbf{U}\,\mathbf{U}^{\dagger} = \mathrm{e}^{i\mathbf{H}}\mathrm{e}^{-i\mathbf{H}^{\dagger}} = \mathbf{I}$ we have $\mathrm{e}^{i\mathbf{H}} = \mathrm{e}^{i\mathbf{H}^{\dagger}}$, which implies $\mathbf{H} = \mathbf{H}^{\dagger}$. Also, from $\det \mathbf{U} = 1$, we can show that $\mathrm{Tr}\,\mathbf{H} = 0$. Consider $\det(\mathrm{e}^{i\mathbf{H}}) = \det(\mathbf{R}\,\mathbf{R}^{-1}\,\mathrm{e}^{i\mathbf{H}}) = \det(\mathbf{R}\,\mathrm{e}^{i\mathbf{H}}\,\mathbf{R}^{-1})$, using the fact that $\det(\mathbf{R}_1\,\mathbf{R}_2) = \det(\mathbf{R}_2\,\mathbf{R}_1) = \det(\mathbf{R}_1)\det(\mathbf{R}_2)$ for any square matrix $\mathbf{R}_j$. Then use:

$$\mathbf{R}\,\mathrm{e}^{i\mathbf{H}}\,\mathbf{R}^{-1} = \mathbf{R}\sum_{n=0}^{\infty}\frac{(i\,\mathbf{H})^n}{n!}\,\mathbf{R}^{-1} = \sum_{n=0}^{\infty}\frac{(i\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1})^n}{n!} = \mathrm{e}^{i\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1}}\,, \tag{1.16}$$

[3] the term "*special*" signifies the fact that any matrix element $\mathbf{U} \in SU(3)$ has a unit determinant $\det \mathbf{U} = 1$.

[4] The exponential of any matrix $\mathbf{A}$ is defined by the exponential series:

$$\mathrm{e}^{\mathbf{A}} = \sum_{n=0}^{\infty}\frac{1}{n!}\,\mathbf{A}^n = \mathbf{I} + \mathbf{A} + \frac{1}{2}\,\mathbf{A}^2 + \ldots$$

to obtain:

$$\det(e^{i\mathbf{H}}) = \det(e^{i\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1}})\,. \tag{1.17}$$

Now if we take $\mathbf{R}$ to be the matrix that diagonalizes the 3×3 matrix $\mathbf{H}$, which is always possible, we then arrive at:

$$\begin{aligned}\det(e^{i\mathbf{H}}) &= \det\begin{pmatrix} e^{i(\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1})_{11}} & 0 & 0 \\ 0 & e^{i(\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1})_{22}} & 0 \\ 0 & 0 & e^{i(\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1})_{33}} \end{pmatrix} = \prod_{j=1}^{3} e^{i(\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1})_{jj}} \\ &= e^{i\sum_{j=1}^{3}(\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1})_{jj}} = e^{i\mathrm{Tr}(\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1})} = e^{i\mathrm{Tr}(\mathbf{R}^{-1}\mathbf{R}\mathbf{H})} = e^{i\mathrm{Tr}(\mathbf{H})}\,, \end{aligned} \tag{1.18}$$

where $(\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1})_{jj}$ denotes the diagonal elements of the diagonal matrix $\mathbf{R}\,\mathbf{H}\,\mathbf{R}^{-1}$. This shows that the requirement $\det(e^{i\mathbf{H}}) = 1$ implies $\mathrm{Tr}(\mathbf{H}) = 0$, completing our argument.

The $SU(3)$ group has only eight generators T_a $(a = 1, 2, \ldots, 8)$, satisfying the commutation relations:

$$[T_a, T_b] = i f_{abc}\, T_c\,, \tag{1.19}$$

where f_{abc} are real constants completely antisymmetric in a, b and c, called the structure constants of the group. A representation for such generators is provided by the eight 3×3 Gell-Mann matrices $\mathcal{T}_a$, which are hermitean and traceless, giving [2]:

$$T_a = \frac{1}{2}\,\mathcal{T}_a\,, \tag{1.20}$$

where

$$\begin{aligned} \mathcal{T}_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{T}_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{T}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{T}_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \\ \mathcal{T}_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \mathcal{T}_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathcal{T}_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \mathcal{T}_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \end{aligned} \tag{1.21}$$

By convention, the $SU(3)$ generators (1.20) are normalized according to:

$$\mathrm{Tr}(T_a\, T_b) = \frac{1}{4}\,\mathrm{Tr}(\mathcal{T}_a\, \mathcal{T}_b) = \frac{1}{2}\,\delta_{ab}\,. \tag{1.22}$$

By multiplying (1.19) with T_s and taking the trace, keeping in mind (1.22), we simply arrive at:

$$f_{abs} = -2i\,\mathrm{Tr}(T_s\,[T_a, T_b]) = -2i\,[\,\mathrm{Tr}(T_s T_a T_b) - \mathrm{Tr}(T_s T_b T_a)\,]\,. \tag{1.23}$$

By using the cyclic property of traces, we can verify easily that f_{abs} is indeed totally antisymmetric. The non-vanishing values for (1.23) are found to be [5]:

$$\begin{aligned} &f_{123} = 1, \\ &f_{147} = -f_{156} = f_{246} = f_{257} = f_{345} = -f_{367} = \frac{1}{2}\,, \\ &f_{458} = f_{678} = \frac{\sqrt{3}}{2}\,. \end{aligned} \tag{1.24}$$

Since not all of the structure constants f_{abc} are zeros, the group is obviously *non*-Abelian. Another important relation of the structure constants of the $SU(N)$ group is:

$$\sum_{c,d=1}^{N^2-1} f_{acd}\, f_{bcd} = N\,\delta_{ab}\,. \tag{1.25}$$

The eight generators $T_a = \mathcal{T}_a/2$ form a set of linearly independent 3×3 traceless Hermitian matrices. Hence, we can expand the matrix $\mathbf{H}$ in (1.15), being traceless and Hermitian, as a linear combination of these generators, rewriting (1.15) as:

$$\mathbf{U} = \mathrm{e}^{i\boldsymbol{\theta}}\,, \qquad \boldsymbol{\theta} = \theta^a\,\mathcal{T}_a/2\,, \tag{1.26}$$

where the components θ^a are arbitrary real parameters, which we may allow them to depend on space-time, and $\theta^a\mathcal{T}_a$ denotes the sum[5] $\sum_{a=1}^{8}\theta^a\mathcal{T}_a$. In (1.26), $\mathbf{U}$ represents a generic $SU(3)$ element which operates on a 3-dimensional column vector space, called the fundamental representation of the $SU(3)$. The number of independent parameters θ^a needed to characterize the group element $\mathbf{U} = \mathbf{U}(\theta^1, \ldots, \theta^8)$ is known as the order of the

[5]N.B. Throughout this thesis we shall adopt the Einstein summation convention.

group, which is $N^2 - 1$ in the case of $SU(N)$ group. This number is always equal to the number of the group generators.

Now, we are in the right position to start the construction of the QCD Lagrangian by applying the gauge principle to the free fermionic Dirac theory in a way analogous to QED. In the absence of any interactions, the Lagrangian for a particular flavour of a quark assumes the form:

$$\begin{aligned}\mathcal{L} = &\overline{\psi}_R(x)(i\gamma^\mu\partial_\mu - m)\psi_R(x) + \overline{\psi}_B(x)(i\gamma^\mu\partial_\mu - m)\psi_B(x) \\ &+ \overline{\psi}_G(x)(i\gamma^\mu\partial_\mu - m)\psi_G(x)\,,\end{aligned} \tag{1.27}$$

where $\psi_R(x)$, $\psi_B(x)$ and $\psi_G(x)$ each denotes a 4-component Dirac spinor for the relevant colour and $\overline{\psi}_R(x) = \psi_R^\dagger(x)\gamma^0$, $\overline{\psi}_B(x) = \psi_B^\dagger(x)\gamma^0$ and $\overline{\psi}_G(x) = \psi_G^\dagger(x)\gamma^0$ are the corresponding adjoint spinors. Unlike QED, the Lagrangian of a free quark (1.27) is a sum of three free Dirac Lagrangians because each flavour of a quark comes in three colour charges. By introducing the colour triplet notation for a particular quark flavour:

$$\Psi(x) = \begin{pmatrix}\psi_R(x)\\ \psi_B(x)\\ \psi_G(x)\end{pmatrix}\,, \qquad \overline{\Psi}(x) = \begin{pmatrix}\overline{\psi}_R(x) & \overline{\psi}_B(x) & \overline{\psi}_G(x)\end{pmatrix}\,, \tag{1.28}$$

we simplify the form of (1.27) as:

$$\mathcal{L} = \overline{\Psi}(x)(i\gamma^\mu\partial_\mu - m)\Psi(x)\,. \tag{1.29}$$

This looks just like the original free Dirac Lagrangian (1.1), only $\Psi(x)$ now stands for a column vector with three components, each of which represents the usual 4-component Dirac spinor.

A quick inspection of the Lagrangian (1.29) shows that it is invariant under the constant phase transformation of the colour triplet:

$$\begin{aligned}\Psi(x) \to \Psi'(x) &= \mathbf{U}\Psi(x) = \mathrm{e}^{i\boldsymbol{\theta}}\,\Psi(x)\,,\\ \overline{\Psi}(x) \to \overline{\Psi}'(x) &= \overline{\Psi}(x)\mathbf{U}^\dagger = \overline{\Psi}(x)\,\mathrm{e}^{-i\boldsymbol{\theta}}\,.\end{aligned} \tag{1.30}$$

However, if we turn this global phase transformation into a local one by simply allowing $\boldsymbol{\theta} = (\theta^1, \ldots, \theta^8)$ to be space-time dependent, i.e. $\partial_\mu \theta^a \neq 0$, the Lagrangian (1.29) ceases to preserve gauge invariance. In analogy with QED, to obtain a local gauge invariant Lagrangian, we have to modify (1.29) according to the following gauge prescription:

1. replace the gradient ∂_μ in (1.29) with the covariant derivative:

$$\boldsymbol{D}_\mu = \mathbf{I}\,\partial_\mu + ig\,\mathbf{A}_\mu\,, \tag{1.31}$$

which is now a 3×3 matrix operator, where g is a coupling constant, the *non*-Abelian counterpart of the electric charge in QED, and $\mathbf{A}_\mu$ is a 3×3 matrix defined in terms of eight gauge fields A^a_μ, equal in number to the generators $\mathcal{T}_a/2$:

$$\mathbf{A}_\mu = \frac{1}{2}\,A^a_\mu\,\mathcal{T}_a = \frac{1}{2}\begin{pmatrix} A^3_\mu + \frac{1}{\sqrt{3}}A^8_\mu & A^1_\mu - iA^2_\mu & A^4_\mu - iA^5_\mu \\ A^1_\mu + iA^2_\mu & -A^3_\mu + \frac{1}{\sqrt{3}}A^8_\mu & A^6_\mu - iA^7_\mu \\ A^4_\mu + iA^5_\mu & A^6_\mu + iA^7_\mu & -\frac{2}{\sqrt{3}}A^8_\mu \end{pmatrix}; \tag{1.32}$$

2. assign to the gauge field matrix $\mathbf{A}_\mu(x)$ a transformation rule such that $\boldsymbol{D}_\mu\Psi$ transforms like Ψ itself:

$$\boldsymbol{D}_\mu\Psi \to [\boldsymbol{D}_\mu\Psi]' \equiv \boldsymbol{D}'_\mu\Psi' = \mathbf{U}\,\boldsymbol{D}_\mu\Psi = \mathrm{e}^{i\boldsymbol{\theta}(x)}\,\boldsymbol{D}_\mu\Psi\,, \tag{1.33}$$

which implies:

$$\boldsymbol{D}_\mu \to \boldsymbol{D}'_\mu = \mathbf{U}\,\boldsymbol{D}_\mu\,\mathbf{U}^\dagger\,. \tag{1.34}$$

Now, we shall make use of this prescription to determine the required transformation law for the $\mathbf{A}_\mu$ matrix of gauge fields. From (1.33), we have:

$$\boldsymbol{D}'_\mu\Psi' = (\mathbf{I}\,\partial_\mu + ig\,\mathbf{A}'_\mu)\,\mathbf{U}\Psi = \mathbf{U}(\mathbf{I}\,\partial_\mu + ig\,\mathbf{A}_\mu)\,\Psi\,. \tag{1.35}$$

Solving this for $\mathbf{A}'_\mu$, we obtain:

$$\mathbf{A}'_\mu = \mathbf{U}\,\mathbf{A}_\mu\mathbf{U}^\dagger + \frac{i}{g}\,(\partial_\mu\mathbf{U})\mathbf{U}^\dagger\,, \tag{1.36}$$

which, by use of the identity:

$$\partial_\mu(\mathbf{U}\,\mathbf{U}^\dagger) = \mathbf{U}\,\partial_\mu\mathbf{U}^\dagger + (\partial_\mu\mathbf{U})\,\mathbf{U}^\dagger = 0\,, \tag{1.37}$$

reduces to:

$$\mathbf{A}'_\mu = \mathbf{U}\,(\mathbf{A}_\mu - \frac{i}{g}\,\mathbf{I}\,\partial_\mu)\,\mathbf{U}^\dagger = -\frac{i}{g}\,\mathbf{U}\,(\boldsymbol{D}_\mu\mathbf{U}^\dagger)\,. \tag{1.38}$$

For an infinitesimal phase transformation such that:

$$\mathbf{U} \cong \mathbf{I} + \frac{i}{2}\,\theta^a(x)\,\mathcal{T}_a\,, \tag{1.39}$$

we have:

$$\mathbf{A}'_\mu \cong \mathbf{A}_\mu - \frac{1}{2g}\,\mathcal{T}_a\,\partial_\mu\theta^a(x) + \frac{i}{2}\,\theta^a(x)\,[\mathcal{T}_a, \mathbf{A}_\mu]\,, \tag{1.40}$$

or equivalently:

$$\mathrm{A}'^a_\mu(x)\mathcal{T}_a \cong \mathrm{A}^a_\mu(x)\,\mathcal{T}_a - \frac{1}{g}\,\mathcal{T}_a\,\partial_\mu\theta^a(x) - f_{abs}\,\theta^a(x)\,\mathrm{A}^b_\mu(x)\,\mathcal{T}_s\,. \tag{1.41}$$

If we now multiply both sides of (1.41) by $\mathcal{T}_c$ and take the trace using (1.22), we obtain the infinitesimal gauge transformations of the bosonic vector fields $\mathrm{A}^c_\mu(x)$:

$$\mathrm{A}^c_\mu(x) \to \mathrm{A}'^c_\mu(x) \cong \mathrm{A}^c_\mu(x) - \frac{1}{g}\,\partial_\mu\theta^c(x) - f_{abc}\,\theta^a(x)\,\mathrm{A}^b_\mu(x)\,. \tag{1.42}$$

By comparing (1.42) with the corresponding expression for photons (1.8), we see that the third term in (1.42) makes the main difference between the two expressions, its dependence on f_{abc} shows explicitly that it is a consequence of the *non*-Abelian symmetry. Noting that $\mathrm{A}^a_\mu(x) = \mathrm{Tr}\,(\mathcal{T}_a\,\mathbf{A}_\mu)$, the exact gauge transformation law for the gauge fields $\mathrm{A}^a_\mu(x)$ can be extracted from (1.38) as:

$$\mathrm{A}^a_\mu(x) \to \mathrm{A}'^a_\mu(x) = -\frac{i}{g}\,\mathrm{Tr}\,(\mathcal{T}_a\,[\mathbf{U}\,\boldsymbol{D}_\mu\mathbf{U}^\dagger])\,. \tag{1.43}$$

So far we have manged to construct from (1.29) a locally $SU(3)$ gauge invariant Lagrangian of the form:

$$\mathcal{L} = \overline{\Psi}(x)(i\gamma^\mu\boldsymbol{D}_\mu - m\,\mathbf{I})\Psi(x) = \overline{\Psi}\,(i\gamma^\mu\partial_\mu - m)\Psi - \frac{g}{2}\,(\overline{\Psi}\,\gamma^\mu\mathcal{T}_a\Psi)\,\mathrm{A}^a_\mu\,. \tag{1.44}$$

The cost of achieving this has been the introduction of eight vector fields A^a_μ, transforming according to (1.43). As these fields are meant to represent the gluons, we should therefore include their kinetic energy terms in (1.44), demanding that they are also gauge invariant. By analogy with QED, we need to find out an appropriate generalization of the photon kinetic energy term $-F_{\mu\nu}F^{\mu\nu}/4$ for the gluons in QCD. We begin by noting that in QED the vector field tensor $F_{\mu\nu}$ can be expressed in terms of the covariant derivative (1.7) as:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \equiv -\frac{i}{e}\left[D_\mu, D_\nu\right]. \tag{1.45}$$

This motivates us to identify the *non*-Abelian $SU(3)$ counterpart as:

$$\mathbf{F}_{\mu\nu} = \partial_\mu \mathbf{A}_\nu - \partial_\nu \mathbf{A}_\mu + ig\left[\mathbf{A}_\mu, \mathbf{A}_\nu\right] \equiv -\frac{i}{g}\left[\boldsymbol{D}_\mu, \boldsymbol{D}_\nu\right], \tag{1.46}$$

which can be expressed in terms of an octet of field strength tensors $F^a_{\mu\nu}(x)$ as:

$$\mathbf{F}_{\mu\nu}(x) = \frac{1}{2}\, F^a_{\mu\nu}(x)\, \mathcal{T}_a\,, \tag{1.47}$$

where

$$F^a_{\mu\nu}(x) = \partial_\mu \mathrm{A}^a_\nu(x) - \partial_\nu \mathrm{A}^a_\mu(x) - g\, f_{abc}\, \mathrm{A}^b_\mu(x)\, \mathrm{A}^c_\nu(x)\,. \tag{1.48}$$

Here, (1.46) transforms under (1.36) as:

$$\mathbf{F}_{\mu\nu} \to \mathbf{F}'_{\mu\nu} = \mathbf{U}\,\mathbf{F}_{\mu\nu}\mathbf{U}^\dagger\,, \tag{1.49}$$

indicating the non-invariance of $\mathbf{F}_{\mu\nu}$ under the gauge transformation (1.36). However, if we consider the Lorentz scalar quantity $\mathrm{Tr}\,(\mathbf{F}_{\mu\nu}\mathbf{F}^{\mu\nu})$ we can see from the cyclic property of the trace that it is gauge invariant under (1.36). Hence, we define the locally gauge invariant Lagrangian describing the kinetic energy of the gluons to be:

$$\mathcal{L}_{YM} = -\frac{1}{2}\,\mathrm{Tr}\,(\mathbf{F}_{\mu\nu}\mathbf{F}^{\mu\nu}) = -\frac{1}{4}\, F^a_{\mu\nu}(x) F^{a\,\mu\nu}(x)\,. \tag{1.50}$$

This is clearly the generalization of the photon kinetic Lagrangian in QED. It is well known as the pure $SU(3)$ Yang-Mills Lagrangian.

Now, we can write the *non*-Abelian gauge invariant Lagrangian of the strong colour

interactions in QCD as:

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F^{a\,\mu\nu} + \overline{\Psi}\,(i\gamma^\mu \partial_\mu - m)\Psi - \frac{g}{2}\,(\overline{\Psi}\,\gamma^\mu \mathcal{T}_a \Psi)\,\mathrm{A}^a_\mu\,. \tag{1.51}$$

The first term in (1.51) imparts a crucial new property to QCD because it includes terms such as:

$$g\,f_{abc}\,\mathrm{A}^b_\mu(x)\,\mathrm{A}^c_\nu(x)\partial^\mu \mathrm{A}^{a\,\nu}(x) \quad \text{and} \quad -\frac{g^2}{4}\,f_{abc}\,f_{ade}\,\mathrm{A}^b_\mu(x)\,\mathrm{A}^c_\nu(x)\mathrm{A}^{d\mu}(x)\mathrm{A}^{e\nu}(x)\,, \tag{1.52}$$

which clearly indicate that the gluon fields are self-interacting through three- and four-leg vertices, respectively. This reflects the fact that unlike QED the gauge fields in QCD, identified with gluons, carry colour charges.

So far, we have considered only one type or flavour of a quark. It is however not difficult to show that for a number of quark flavours n_f the QCD Lagrangian assumes the form:

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F^{a\,\mu\nu} + \sum_{f=1}^{n_f} \overline{\Psi}_f\,(i\gamma^\mu \partial_\mu - m_f)\Psi_f - \frac{g}{2} \sum_{f=1}^{n_f} (\overline{\Psi}_f\,\gamma^\mu \mathcal{T}_a \Psi_f)\,\mathrm{A}^a_\mu\,, \tag{1.53}$$

where Ψ_f and m_f denote the colour field triplet and the mass of the quark flavour (labelled by f) respectively.

1.2 Asymptotic freedom in QCD

1.2.1 Notation and Conventions

In this section, our notation and conventions will be slightly different from those used in the previous section. Following Refs. [6,7], we redefine the generators of the $SU(N)$ group, in the fundamental representation, by the antihermitian matrices:

$$t_a = -i\,T_a\,, \qquad t_a^\dagger = -t_a, \tag{1.54}$$

such that:

$$[t_a, t_b] = f_{abc}\,t_c\,, \qquad \mathrm{Tr}\,(t_a\,t_b) = -\frac{\delta_{ab}}{2}\,. \tag{1.55}$$

Note that the matrices T_a in (1.54) are hermitian and traceless, and reduce to (1.20) in the case of the $SU(3)$ group. In terms of these antihermitian generators, the gauge fields, field strength tensors and the group elements of the $SU(N)$ group are re-expressed as:

$$\tilde{A}_\mu(x) = \tilde{A}^a_\mu(x)\, t_a\,, \quad \tilde{F}_{\mu\nu}(x) = \tilde{F}^a_{\mu\nu}(x)\, t_a\,, \quad U(x) = \mathrm{e}^{\tilde{\theta}(x)}\,, \tag{1.56}$$

with $\tilde{\theta}(x) = \tilde{\theta}^a(x)\, t_a$. Here $\tilde{A}_\mu(x)$, $\tilde{F}_{\mu\nu}(x)$ and $\tilde{\theta}(x)$ are related to our previous notation in section (1.1) via the simple relations:

$$\tilde{A}_\mu(x) = igA^a_\mu(x)\, T_a\,, \qquad \tilde{F}_{\mu\nu}(x) = igF^a_{\mu\nu}(x)\, T_a\,, \qquad \tilde{\theta}(x) = i\,\theta^a(x)\, T_a\,. \tag{1.57}$$

Notice that the coupling constant g is now lumped into the gauge field components $\tilde{A}^a_\mu(x) = -g\, A^a_\mu(x)$, resulting in $\tilde{F}^a_{\mu\nu}(x) = -g\, F^a_{\mu\nu}(x)$. Under these conventions, various expressions can be written in more compact forms. For example, the covariant derivative (in the fundamental representation), the field strength tensor and the gauge field transformation will now read as:

$$D_\mu = \partial_\mu + \tilde{A}_\mu\,, \tag{1.58}$$

$$\tilde{F}_{\mu\nu}(x) = [D_\mu, D_\nu] = \partial_\mu \tilde{A}_\nu - \partial_\nu \tilde{A}_\mu + [\tilde{A}_\mu, \tilde{A}_\nu]\,, \tag{1.59}$$

$$\tilde{A}_\mu \to \tilde{A}'_\mu = U\,(\partial_\mu + \tilde{A}_\mu)\,U^\dagger\,. \tag{1.60}$$

In an n-dimensional Euclidean space-time, the action of the pure $SU(N)$ Yang-Mills theory is given by:

$$S[\tilde{A}_\mu] = S_E[\tilde{A}_\mu]/g^2\,, \tag{1.61}$$

where

$$S_E[\tilde{A}_\mu] = -\frac{1}{2}\int d^n x\ \mathrm{Tr}\,(\tilde{F}_{\mu\nu}(x)\tilde{F}_{\mu\nu}(x)) = \frac{1}{4}\int d^n x\ \tilde{F}^a_{\mu\nu}(x)\tilde{F}^a_{\mu\nu}(x)\,. \tag{1.62}$$

For brevity, from now on we shall omit all the tildes in our notation. So, in what follows we will use $A_\mu = A^a_\mu\, t_a$, $F_{\mu\nu} = F^a_{\mu\nu}\, t_a$ and $\theta = \theta^a\, t_a$ to denote the relevant quantities in (1.56). Now, we shall introduce the following definitions: if the covariant derivative D_μ acts on the adjoint group space, i.e. on elements containing the matrix generators t_a, then

we identify D_μ as:

$$D_\mu = \partial_\mu + [A_\mu, \ ], \tag{1.63}$$

such that:

$$D_\mu V = \partial_\mu V + [A_\mu, V], \qquad \text{for any} \quad V = V^a(x)\, t_a\,. \tag{1.64}$$

In matrix components, we have:

$$D^{ab}_\mu = \delta_{ab}\,\partial_\mu + A^c_\mu\, L^c_{ab}\,, \qquad (D_\mu V)^a \equiv D^{ab}_\mu V^b = \partial_\mu V^a + A^c_\mu\, L^c_{ab}\, V^b\,, \tag{1.65}$$

with $L^c_{ab} = -f_{abc}$. Under this convention, we can show that [5]:

$$[D_\mu, D_\nu]V = [F_{\mu\nu}, V]\,, \qquad D_\mu(V_1\, V_2) = (D_\mu\, V_1)\, V_2 + V_1\, D_\mu\, V_2\,, \tag{1.66}$$

where $V_i = V_i^a\, t_a$. Furthermore, we shall denote any field matrix in the adjoint representation by

$$V^{\mathtt{adj}} = V^c(x)\, L^c \iff V^{\mathtt{adj}}_{ab} = V^c(x)\, L^c_{ab}\,, \tag{1.67}$$

where L^a is a square matrix of dimension $N^2 - 1$ and satisfies:

$$[L^a, L^b] = f_{abc}\, L^c\,, \qquad \mathrm{Tr}\,(L^a\, L^b) = -N\,\delta_{ab}\,. \tag{1.68}$$

Here, the matrices L^a for $a = 1, 2, \ldots, N^2 - 1$ are called generators of the $SU(N)$ group in the adjoint representation.

1.2.2 Background field approach to asymptotic freedom

The background field method [6, 8, 9] is a technique for quantizing gauge field theories in the presence of a classical background field normally chosen so that certain symmetries of the generating functionals are restored. Technically, this method makes calculations in gauge theories clearer and more transparent. In this section, we shall use this approach for investigating asymptotic freedom in non-Abelian $SU(N)$ gauge theories with no fermions.

Within the conventional Faddeev-Popov gauge-fixing procedure, the generating functional of pure Yang-Mills fields in 4-dimensional Euclidean space-time assumes the

form [9]:

$$Z = Z_0 \int \mathcal{D}A_\mu \ \triangle_{FP}[A_\mu]\ \delta[\,G[A_\mu]\,]\ \mathrm{e}^{-S_E[A_\mu]/g^2}\,, \tag{1.69}$$

where Z_0 is a normalization constant, $\mathcal{D}A_\mu$ is a local gauge-invariant measure defined as:

$$\mathcal{D}A_\mu = \prod_{\mu=0}^{3} \prod_{a=1}^{N^2-1} \prod_{x} dA_\mu^a(x)\,, \tag{1.70}$$

and $\delta[\,G[A_\mu]\,]$ represents the δ-functional which is a product of the usual 4-dimensional Dirac δ-functions:

$$\delta[\,G[A_\mu]\,] = \prod_{a=1}^{N^2-1} \prod_{x} \delta(\,G^a[A_\mu](x)\,)\,, \tag{1.71}$$

with $G^a[A_\mu](x)$ being the $a\,th$ x-dependent component of the arbitrary gauge-fixing function $G[A_\mu]$. For example, $G^a[A_\mu](x) = \partial_\mu A_\mu^a(x)$ is a common choice called the Lorentz gauge. In (1.69), the δ-functional imposes the so-called gauge-fixing condition $G^a[A_\mu](x) = 0$, which restricts the functional integration over the field configurations. By $\triangle_{FP}[A_\mu]$ we denote the Faddeev-Popov determinant in both space-time and group indices:

$$\triangle_{FP}[A_\mu] = \det(M^{ab}(x,y))\,, \tag{1.72}$$

where the matrix element $M^{ab}(x,y)$ is given by:

$$M^{ab}(x,y) = \left.\frac{\delta G^a[\,{}^\theta A_\mu](x)}{\delta\theta^b(y)}\right|_{\theta^b=0} = \int d^4z\, \frac{\delta G^a[\,{}^\theta A_\mu](x)}{\delta\,{}^\theta A_\nu^c(z)}\, \left.\frac{\delta\,{}^\theta A_\nu^c(z)}{\delta\theta^b(y)}\right|_{\theta^b=0}. \tag{1.73}$$

Here, ${}^\theta A_\mu(x)$ is the gauge transformed field (1.60):

$${}^\theta A_\mu(x) = \mathrm{e}^{\theta(x)}\,(\partial_\mu + A_\mu(x))\,\mathrm{e}^{-\theta(x)} = A_\mu(x) - \partial_\mu\theta(x) - [A_\mu, \mathrm{e}^\theta]\,\mathrm{e}^{-\theta(x)}\,. \tag{1.74}$$

Since $\triangle_{FP}[A_\mu]$ is evaluated at $\theta(x) = 0$, it is enough to consider only infinitesimal gauge transformations $U(x) = I + \theta(x)$, giving:

$${}^\theta A_\mu(x) = A_\mu(x) - D_\mu\theta(x)\,. \tag{1.75}$$

Now, the basic idea of the background field method is to split the gauge field $A_\mu(x)$ in

(1.69) into a classical background field $B_\mu(x)$ and a fluctuating quantum field $\omega_\mu(x)$:

$$A_\mu(x) = B_\mu(x) + g_0\,\omega_\mu(x), \qquad g_0 = g/q\,, \tag{1.76}$$

where q is a mass scale parameter. We will treat the classical part as a fixed field configuration and the fluctuating part as the integration variable of the functional integral. By regarding $B_\mu(x)$ as fixed, the invariance of the Euclidean action $S_E[A_\mu]$ under the infinitesimal gauge transformation (1.75) implies the invariance of $S_E[B_\mu + g_0\,\omega_\mu]$ under the following gauge transformation:

$${}^\theta\omega_\mu(x) = \omega_\mu(x) - \frac{1}{g_0}\,\mathfrak{D}_\mu\theta(x) - [\omega_\mu(x), \theta(x)]\,, \tag{1.77}$$

or alternatively (in components):

$${}^\theta\omega^a_\mu(x) = \omega^a_\mu(x) - \frac{1}{g_0}\,\mathfrak{D}^{ab}_\mu\theta^b(x) + f_{abc}\;\omega^c_\mu(x)\,\theta^b(x)\,, \tag{1.78}$$

where $\mathfrak{D}^{ab}_\mu$ is the matrix components of the covariant derivative $\mathfrak{D}_\mu$ with respect to the background field in the adjoint representation:

$$\mathfrak{D}^{ab}_\mu = \delta_{ab}\,\partial_\mu + B^c_\mu(x)\,L^c_{ab}\,. \tag{1.79}$$

The gauge-fixing condition which is commonly used in the background field method reads as:

$$G^a[A_\mu, B_\mu](x) = q^{-2}\left(\mathfrak{D}^{ab}_\mu A^b_\mu(x) - \partial_\mu B^a_\mu(x)\right) = 0\,, \tag{1.80}$$

which, under the change of variables (1.76), reduces to:

$$\widetilde{G}^a[\omega_\mu, B_\mu](x) = g_0\,q^{-2}\,\mathfrak{D}^{ab}_\mu\omega^b_\mu(x) = 0\,. \tag{1.81}$$

This may seem a rather unusual gauge choice as it depends on an extra field $B_\mu(x)$. However, it is perfectly acceptable and known as the background field gauge. The mass scale parameter q in the gauge-fixing function is introduced so that the Faddeev-Popov determinant remains dimensionless.

Now, if we change variables in (1.69) using (1.76) we obtain:

$$Z = \widetilde{Z}[B_\mu] = \widetilde{Z}_0 \int \mathcal{D}\omega_\mu \; \widetilde{\Delta}_{FP}[\omega_\mu] \; \delta[\, g_0\, q^{-2}\, \mathfrak{D}_\mu \omega_\mu \,] \; \mathrm{e}^{-S_E[B_\mu + g_0\, \omega_\mu]/g^2} \,, \tag{1.82}$$

where $\delta[\, g_0\, q^{-2}\, \mathfrak{D}_\mu \omega_\mu \,] = \prod_{a=1}^{N} \delta[\, g_0\, q^{-2}\, \mathfrak{D}_\mu^{ab} \omega_\mu^b \,]$ and

$$\begin{aligned} \widetilde{\Delta}_{FP}[\omega_\mu] &= \det \left(\frac{\delta \widetilde{G}^a[\, {}^\theta\omega_\mu, B_\mu](x)}{\delta \theta^b(y)} \right) = \det \left(g_0\, q^{-2}\, \mathfrak{D}_\mu^{ac}\, \frac{\delta\, {}^\theta\omega_\mu^c(x)}{\delta \theta^b(y)} \right) \\ &= \det \left(-q^{-2}\, \mathfrak{D}_{ab}^2 - g_0\, q^{-2}\, f_{bce}\, \mathfrak{D}_\mu^{ac}\, \omega_\mu^e(x) \right) . \end{aligned} \tag{1.83}$$

Here $\mathfrak{D}_{ab}^2 = \mathfrak{D}_\mu^{ac}\, \mathfrak{D}_\mu^{cb}$.

Consider the following class of gauge conditions [9]:

$$\widetilde{G}^a[\omega_\mu, B_\mu, C](x) = g_0\, q^{-2}\, \mathfrak{D}_\mu^{ab} \omega_\mu^b(x) - C^a(x) = 0 \,, \tag{1.84}$$

where $C^a(x)$ is an arbitrary function of a space-time point and $\widetilde{G}^a[\omega_\mu, B_\mu, 0](x) = \widetilde{G}^a[\omega_\mu, B_\mu](x)$. For all gauge conditions belonging to this class, the Faddeev-Popov determinant in (1.82) is the same because $C^a(x)$ is unaffected by the gauge transformation from ω_μ to ${}^\theta\omega_\mu$. This allows us to replace the δ-functional in (1.82) by some other functional depending on the gauge-fixing function $\widetilde{G}^a[\omega_\mu, B_\mu](x)$ in a more convenient way for practical calculations.

Having started with the gauge condition (1.84) for $C^a(x) \neq 0$, instead of (1.81), we would have obtained:

$$Z = \widetilde{Z}[B_\mu] = \widetilde{Z}_0 \int \mathcal{D}\omega_\mu \; \widetilde{\Delta}_{FP}[\omega_\mu] \; \delta[\, g_0\, q^{-2}\, \mathfrak{D}_\mu \omega_\mu - C \,] \; \mathrm{e}^{-S_E[B_\mu + g_0\, \omega_\mu]/g^2} \,. \tag{1.85}$$

Being gauge-invariant, this quantity is obviously independent of $C(x)$. Hence, by integrating (1.85) functionally over $C(x)$ with an arbitrary weight functional $W[C]$, we obtain, on the left hand side, Z times a constant $\int \mathcal{D}C \; W[C]$ which can be lumped into the normalization factor $\widetilde{Z}_0$, while, on the right hand side, the integration over $C(x)$ can be performed trivially with the help of the δ-functional, giving:

$$Z = \widetilde{Z}[B_\mu] = \widetilde{Z}_0' \int \mathcal{D}\omega_\mu \; \widetilde{\Delta}_{FP}[\omega_\mu] \; W[\, g_0\, q^{-2}\, \mathfrak{D}_\mu \omega_\mu \,] \; \mathrm{e}^{-S_E[B_\mu + g_0\, \omega_\mu]/g^2} \,. \tag{1.86}$$

Here, $\widetilde{Z}_0' = \widetilde{Z}_0 / \int \mathcal{D}C\, W[C]$.

A popular choice for the weight functional $W[C]$ is given by:

$$W[C] = \exp\left(\frac{q^2}{g_0^2\,\xi}\int d^4x\ \mathrm{Tr}(C(x)^2)\right) = \exp\left(-\frac{1}{2}\,\frac{q^2}{g_0^2\,\xi}\int d^4x\ C^a(x)^2\right), \tag{1.87}$$

where ξ is an arbitrary real number. In this expression, q^2/g_0^2 is included so that the exponent remains dimensionless. Using (1.87) in (1.86), we obtain:

$$Z = \widetilde{Z}[B_\mu] = \widetilde{Z}_0' \int \mathcal{D}\omega_\mu\ \widetilde{\Delta}_{FP}[\omega_\mu]\ \mathrm{e}^{-S_E[B_\mu + g_0\,\omega_\mu]/g^2}\mathrm{e}^{-S_{GF}[\omega_\mu]}\,, \tag{1.88}$$

where the gauge-fixing action $S_{GF}[\omega_\mu]$ is given by:

$$S_{GF}[\omega_\mu] = -\frac{1}{q^2\xi}\int d^4x\ \mathrm{Tr}([\mathfrak{D}_\mu\omega_\mu(x)]^2) = \frac{1}{2}\,\frac{1}{q^2\xi}\int d^4x\ \mathfrak{D}_\mu^{ab}\omega_\mu^b(x)\ \mathfrak{D}_\nu^{ac}\omega_\nu^c(x). \tag{1.89}$$

By making use of the fact that $(\mathfrak{D}_\mu\,\omega_\mu)^2 = \mathfrak{D}_\mu(\omega_\mu\mathfrak{D}_\nu\omega_\nu) - \omega_\mu\mathfrak{D}_\mu\mathfrak{D}_\nu\omega_\nu$ and:

$$\int d^4x\ \mathrm{Tr}\left(\mathfrak{D}_\mu(\omega_\mu\,\mathfrak{D}_\nu\omega_\nu)\right) = 0\,, \tag{1.90}$$

we can rewrite (1.89) as:

$$S_{GF}[\omega_\mu] = \frac{1}{q^2\xi}\int d^4x\ \mathrm{Tr}(\omega_\mu\mathfrak{D}_\mu\mathfrak{D}_\nu\omega_\nu) = -\frac{1}{2}\,\frac{1}{q^2\xi}\int d^4x\ \omega_\mu^a(x)\,\mathfrak{D}_\mu^{ab}\,\mathfrak{D}_\nu^{bc}\,\omega_\nu^c(x). \tag{1.91}$$

1.2.3 One-loop approximation

We shall evaluate the functional integral (1.88) to one-loop order, which corresponds to the omission of terms non-quadratic in the fluctuating field $\omega_\lambda(x)$. We begin by expanding the Euclidean action $S_E[B_\lambda + g_0\,\omega_\lambda]$ in a functional Taylor series about $B_\lambda(x)$, retaining only the first three leading terms:

$$\begin{aligned} S_E[B_\lambda + g_0\,\omega_\lambda] = S_E[B_\lambda] &+ g_0\int d^4x\ \omega_\mu^a(x)\ \frac{\delta S_E[B_\lambda]}{\delta B_\mu^a(x)} \\ &+ \frac{g_0^2}{2}\int d^4x\,d^4y\ \omega_\mu^a(x)\ \frac{\delta^2 S_E[B_\lambda]}{\delta B_\mu^a(x)\,\delta B_\nu^b(y)}\ \omega_\nu^b(y)\ +\ \mathrm{O}(g_0^3\,\omega_\lambda^3)\,. \end{aligned} \tag{1.92}$$

Here, we have:

$$\frac{\delta S_E[B_\lambda]}{\delta B^a_\mu(x)} = \frac{1}{2}\int d^4y\, F^b_{\nu\lambda}(y)\frac{\delta F^b_{\nu\lambda}(y)}{\delta B^a_\mu(x)} = \int d^4y\, F^b_{\nu\mu}(y)\, \mathfrak{D}^{ba}_\nu \delta(y-x) = j^a_\mu(x)\,, \tag{1.93}$$

where $j^a_\mu(x) = \mathfrak{D}^{ab}_\nu F^b_{\mu\nu}(x)$, known as the *a-th* component of the non-Abelian vector current $j_\mu(x) = \mathfrak{D}_\nu F_{\mu\nu}(x)$. Note that the field strength tensor $F_{\mu\nu}(x)$ is now defined with respect to the background field $B_\mu(x)$. Also, in (1.92) we have:

$$\frac{\delta^2 S_E[B_\lambda]}{\delta B^b_\nu(y)\,\delta B^a_\mu(x)} = \frac{\delta j^a_\mu(x)}{\delta B^b_\nu(y)} = \triangle^{ab}_{\mu\nu}\delta(x-y)\,, \tag{1.94}$$

where

$$\triangle^{ab}_{\mu\nu} = -\delta_{\mu\nu}\,\mathfrak{D}^2_{ab} + f_{abc}\,F^c_{\mu\nu}(x) + \mathfrak{D}^{ac}_\nu\,\mathfrak{D}^{cb}_\mu\,, \tag{1.95}$$

which, with the help of the identity $[\mathfrak{D}_\mu, \mathfrak{D}_\nu]_{ab} \equiv F^c_{\mu\nu}\,L^c_{ab}$ in the adjoint representation, we can rewrite as:

$$\triangle^{ab}_{\mu\nu} = -\delta_{\mu\nu}\,\mathfrak{D}^2_{ab} + 2f_{abc}\,F^c_{\mu\nu}(x) + \mathfrak{D}^{ac}_\mu\,\mathfrak{D}^{cb}_\nu\,. \tag{1.96}$$

For simplicity, we choose the background field $B_\mu(x)$ to be the solution of the classical field equation of motion:

$$\mathfrak{D}_\nu F_{\mu\nu}(x) = \partial_\nu F_{\mu\nu}(x) + [B_\nu, F_{\mu\nu}] = 0\,, \tag{1.97}$$

reducing the Taylor expansion in (1.92) to:

$$S_E[B_\mu + g_0\,\omega_\mu] = S_E[B_\mu] + \frac{g_0^2}{2}\int d^4x\;\omega^a_\mu(x)\;\triangle^{ab}_{\mu\nu}\;\omega^b_\nu(x) \;+\; \mathrm{O}(g_0^3\,\omega_\mu^3)\,. \tag{1.98}$$

Substituting this into (1.88), we arrive at:

$$Z = \widetilde{Z}'_0\;\mathrm{e}^{-S_E[B_\mu]/g^2}\int \mathcal{D}\omega_\mu\;\widetilde{\triangle}_{FP}[\omega_\mu]\;\mathrm{e}^{-S_0[\omega_\mu]}\,, \tag{1.99}$$

where

$$S_0[\omega_\mu] = \frac{q^{-2}}{2}\int d^4x\;\omega^a_\mu(x)\,\triangle^{ab}_{0\,\mu\nu}\;\omega^b_\nu(x) \;+\; \mathrm{O}(g)\,, \tag{1.100}$$

with

$$\triangle^{ab}_{0\,\mu\nu} = -\delta_{\mu\nu}\,\mathfrak{D}^2_{ab} + 2f_{abc}\,F^c_{\mu\nu}(x) + (1-1/\xi)\,\mathfrak{D}^{ac}_\mu\,\mathfrak{D}^{cb}_\nu\,. \tag{1.101}$$

Since ξ is a freely adjustable parameter, it is certainly simpler to work with $\xi = 1$. This is called the Feynmann-t'Hooft gauge which will be imposed from now on.

Within the one-loop approximation, the Faddeev-Popov determinant in (1.99) reduces to $\det\left(-q^{-2}\,\mathfrak{D}^2_{ab}\right)$ as can be seen from (1.83). Being independent of the quantum fluctuation $\omega_\mu(x)$, this simplifies the functional integral in (1.99), giving:

$$\begin{aligned} Z &= \widetilde{Z}_0'\ \mathrm{e}^{-S_E[B_\mu]/g^2}\ \det\left(-\mathfrak{D}^2/q^2\right) \int \mathcal{D}\omega_\mu\ \mathrm{e}^{-S_0[\omega_\mu]} \\ &= \mathcal{C}\ \mathrm{e}^{-S_E[B_\mu]/g^2}\ \frac{\det\left(-\mathfrak{D}^2/q^2\right)}{\det\left(\triangle_{0\,\mu\nu}/q^2\right)^{1/2}}\,, \end{aligned} \tag{1.102}$$

where $\mathcal{C}$ is an overall constant independent of q and g. Here, recall that $\mathfrak{D}^2$ and $\triangle_{0\,\mu\nu}$ are operator matrices, in the adjoint representation, given by:

$$\begin{aligned} \mathfrak{D}^2 &= \mathfrak{D}_\mu\,\mathfrak{D}_\mu \qquad \text{with} \qquad \mathfrak{D}_\mu = \mathrm{I}\,\partial_\mu + B^c_\mu(x)\,L^c\,, \\ \triangle_{0\,\mu\nu} &= -\delta_{\mu\nu}\,\mathfrak{D}^2 - 2\,F^{\mathsf{adj}}_{\mu\nu}(x)\,, \end{aligned} \tag{1.103}$$

where $F^{\mathsf{adj}}_{\mu\nu}(x) = F^c_{\mu\nu}(x)\,L^c$ with L^c being a square matrix of order $N^2 - 1$ and elements $L^c_{ab} = -f_{abc}$ and I is a unit matrix. In this representation, $\mathfrak{D}^2_{ab}$ and $\triangle^{ab}_{0\,\mu\nu}$ are the corresponding matrix elements of $\mathfrak{D}^2$ and $\triangle_{0\,\mu\nu}$ respectively. In (1.102), the previous introduction of the arbitrary mass scale parameter q turns out to be necessary for keeping the determinants dimensionless.

1.2.4 ζ−function evaluation of determinants

In this subsection, we shall describe an effective method for evaluating determinants of a certain class of operators by means of a generalized version of the Riemann zeta function [10, 11]. Then, we will apply this method to the two determinants we encountered in (1.102), giving the explicit q-dependence of g by which we observe asymptotic freedom in QCD.

Consider an $N \times N$ operator matrix $\hat{A}$ with real, positive and discrete eigenvalues λ_n such that:

$$\hat{A}\,\Phi_n(x) = \lambda_n\,\Phi_n(x)\,, \qquad \text{for all } n \in \mathbb{N}, \tag{1.104}$$

where $\Phi_n(x)$ is a column matrix with elements $\Phi^a_n(x)$ forming a complete orthonormal

basis:

$$\sum_{a=1}^{N} \int d^4x \; \Phi_n^a(x) \; \Phi_m^{a\,*}(x) = \delta_{nm} \,, \qquad \sum_{n=1}^{\infty} \Phi_n^a(x) \; \Phi_n^{b\,*}(y) = \delta(x-y) \; \delta_{ab} \,. \tag{1.105}$$

Alternatively, in matrix notation, this reads as:

$$\int d^4x \; \mathrm{Tr}\left(\Phi_n(x) \; \Phi_m^\dagger(x) \right) = \delta_{nm} \,, \qquad \sum_{n=1}^{\infty} \Phi_n(x) \; \Phi_n^\dagger(y) = \delta(x-y) \; \mathrm{I} \,, \tag{1.106}$$

where I is an $N \times N$ unit matrix.

The determinant of $\hat{A}$ is defined as the product of its eigenvalues:

$$\det(\hat{A}) = \prod_{n=1}^{\infty} \lambda_n \,. \tag{1.107}$$

This can be expressed in terms of an associated Riemann zeta function:

$$\zeta_{\hat{A}}(s) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n^s} \,. \tag{1.108}$$

By differentiating this once with respect to s, we find that for $s = 0$:

$$\zeta'_{\hat{A}}(0) = -\sum_{n=1}^{\infty} \ln(\lambda_n) = -\ln(\prod_{n=1}^{\infty} \lambda_n) \,, \tag{1.109}$$

which gives:

$$\det(\hat{A}) = \mathrm{e}^{-\zeta'_{\hat{A}}(0)} \,. \tag{1.110}$$

An immediate consequence of (1.108) is that

$$\zeta_{\hat{A}/\mu}(s) = \mu^s \, \zeta_{\hat{A}}(s) \,, \tag{1.111}$$

for any scalar μ, which implies:

$$\zeta'_{\hat{A}/\mu}(0) = \zeta_{\hat{A}}(0) \; \ln(\mu) + \zeta'_{\hat{A}}(0) \,, \tag{1.112}$$

or rather:

$$\det(\hat{A}/\mu) = \mathrm{e}^{-\zeta_{\hat{A}}(0) \; \ln(\mu)} \; \det(\hat{A}) \,. \tag{1.113}$$

Using the integral representation for the Γ-function:

$$\Gamma(s) = \int_0^\infty t^{s-1}\, \mathrm{e}^{-t}\, dt\,, \tag{1.114}$$

we can show that:

$$\zeta_{\hat{A}}(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1}\, \mathrm{Tr}\,(\mathrm{e}^{-t\,\hat{A}})\, dt\,, \tag{1.115}$$

where

$$\mathrm{Tr}\,(\mathrm{e}^{-t\,\hat{A}}) = \sum_{n=1}^{\infty} \mathrm{e}^{-\lambda_n t}\,. \tag{1.116}$$

One way to compute the trace of $\exp(-t\,\hat{A})$ is by considering the kernel $G(x,y;t)$, which satisfies the heat equation:

$$\frac{\partial G(x,y;t)}{\partial t} = -\hat{A}_x\, G(x,y;t)\,, \tag{1.117}$$

and the initial condition $G(x,y;0) = \delta(x-y)$ I. Here, we use $\hat{A}_x$ to indicate that $\hat{A}$ acts on x rather than y or t. The formal solution of (1.117) is given by:

$$G(x,y;t) = \mathrm{e}^{-t\,\hat{A}_x}\, G(x,y;0)\,, \tag{1.118}$$

which, with the help of the initial condition and (1.106), we can write as:

$$G(x,y;t) = \sum_{n=1}^{\infty} \mathrm{e}^{-\lambda_n t}\, \Phi_n(x)\, \Phi_n^\dagger(y)\,. \tag{1.119}$$

By taking the trace of $G(x,x;t)$ in (1.119), integrating with respect to x and using the orthogonality relation in (1.106), we obtain:

$$\mathrm{Tr}\,(\mathrm{e}^{-t\,\hat{A}}) = \int \mathrm{Tr}\,(G(x,x;t))\, dx\,. \tag{1.120}$$

Here $\mathrm{Tr}\,(G(x,x;t)) = \sum_{a=1}^{N} G^{aa}(x,x;t)$, where G^{ab} denotes the matrix elements of G which can be expressed as:

$$G^{ab}(x,y;t) = \sum_{n=1}^{\infty} \mathrm{e}^{-\lambda_n t}\, \Phi_n^a(x)\, \Phi_n^{b\,*}(y)\,. \tag{1.121}$$

Now we shall apply the heat kernel method to our problem, giving a detailed discussion on evaluating the zeta function $\zeta_{\hat{A}}(0)$ for both $\hat{A} = -\mathfrak{D}^2$ and $\hat{A} = \triangle_{0\,\mu\nu}$. We begin by introducing the heat kernels:

$$\mathsf{G}(x,y;t) = \mathrm{e}^{t\mathfrak{D}^2}\,\delta(x-y)\,\mathrm{I}\,, \qquad \mathsf{K}(x,y;t) = \mathrm{e}^{-t\triangle_{0\mu\nu}}\,\delta(x-y)\,\mathrm{I}\,, \tag{1.122}$$

which satisfy the generalized heat equations:

$$\frac{\partial \mathsf{G}(x,y;t)}{\partial t} = \mathfrak{D}^2\,\mathsf{G}(x,y;t)\,, \qquad \frac{\partial \mathsf{K}_{\mu\nu}(x,y;t)}{\partial t} = -\triangle_{0\mu\nu}\,\mathsf{K}_{\mu\nu}(x,y;t)\,, \tag{1.123}$$

subject to the initial conditions:

$$\lim_{t\to 0}\mathsf{G}(x,y;t) = \delta(x-y)\,\mathrm{I}\,, \qquad \lim_{t\to 0}\mathsf{K}_{\mu\nu}(x,y;t) = \delta(x-y)\,\delta_{\mu\nu}\,\mathrm{I}\,, \tag{1.124}$$

in 4-dimensional Euclidean space-time. Here $t \geq 0$ is just an auxiliary variable, not implying time, and I is a unit matrix in the adjoint representation. Following Refs [6,10], the heat kernels $\mathsf{G}(x,y;t)$ and $\mathsf{K}_{\mu\nu}(x,y;t)$ tend to have the following asymptotic expansions for small t:

$$\mathsf{G}(x,y;t) = \frac{1}{16\pi^2\,t^2}\,\mathrm{e}^{-(x-y)^2/4t}\sum_{n=0}^{\infty}\mathsf{a}_n(x,y)\,t^n\,, \tag{1.125}$$

$$\mathsf{K}_{\mu\nu}(x,y;t) = \frac{1}{16\pi^2\,t^2}\,\mathrm{e}^{-(x-y)^2/4t}\sum_{n=0}^{\infty}\mathsf{b}_{n,\mu\nu}(x,y)\,t^n\,. \tag{1.126}$$

The initial conditions (1.124) imply that:

$$\mathsf{a}_0(x,x) = \mathrm{I}\,, \qquad \mathsf{b}_{0,\mu\nu}(x,x) = \delta_{\mu\nu}\,\mathrm{I}\,. \tag{1.127}$$

From the behaviour of $\mathsf{G}(x,y;t)$ and $\mathsf{K}_{\mu\nu}(x,y;t)$ near $t=0$ and the fact that they decay exponentially as $t\to\infty$, we shall show how to analytically extend $\zeta_{-\mathfrak{D}^2}(s)$ and $\zeta_{\triangle_{0\,\mu\nu}}(s)$ to meromorphic functions of s, each with poles only at $s=1$ and $s=2$ and regular at $s=0$. For $\hat{A} = -\mathfrak{D}^2$, we have:

$$\zeta_{-\mathfrak{D}^2}(s) = \int f(x,s)\,d^4x\,, \tag{1.128}$$

where

$$f(x,s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} \operatorname{Tr}\left(\mathsf{G}(x,x;t)\right) dt\,. \tag{1.129}$$

Since $\operatorname{Tr}\left(\mathsf{G}(x,x;t)\right)$ behaves like $1/t^2$ in the neighbourhood of $t=0$, the integral in (1.129) diverges for $s \leq 2$. However, we can still analytically continue $f(x,s)$ to the complex s-plane, using a different integral representation which converges for $\operatorname{Re}\{s\} \geq 0$. This method is known as the $\zeta-$function regularisation.

Consider the special case of $s > 2$ and integrate (1.129) by parts three successive times to obtain:

$$\begin{aligned} f(x,s) = {} & \frac{1}{(s-1)(s-2)} \sum_{n=0}^{2} \frac{(-1)^n}{\Gamma(s-n+1)} t^{s-n} \frac{\partial^{2-n}}{\partial t^{2-n}} t^2 \operatorname{Tr}\left(\mathsf{G}(x,x;t)\right)\Big|_{t=0}^{\infty} \\ & - \frac{1}{s(s-1)(s-2)\Gamma(s)} \int_0^\infty t^s \frac{\partial^3}{\partial t^3} t^2 \operatorname{Tr}\left(\mathsf{G}(x,x;t)\right) dt\,, \end{aligned} \tag{1.130}$$

which, as a consequence of the small and large t-behaviour of $\mathsf{G}(x,x;t)$, reduces to:

$$f(x,s) = -\frac{1}{(s-1)(s-2)\Gamma(s+1)} \int_0^\infty t^s \frac{\partial^3}{\partial t^3} t^2 \operatorname{Tr}\left(\mathsf{G}(x,x;t)\right) dt\,. \tag{1.131}$$

This expression allows us to analytically continue from the positive real interval $s > 2$ to the right half complex plane $\operatorname{Re}\{s\} \geq 0$, giving for $s = 0$ the unique analytic contribution:

$$f(x,0) = \frac{1}{2} \frac{\partial^2}{\partial t^2} t^2 \operatorname{Tr}\left(\mathsf{G}(x,x;t)\right)\Big|_{t=0} = \frac{1}{16\,\pi^2} \operatorname{Tr}\left(\mathsf{a}_2(x,x)\right), \tag{1.132}$$

which, when used in (1.128), leads to:

$$\zeta_{-\mathfrak{D}^2}(0) = \frac{1}{16\,\pi^2} \int \operatorname{Tr}\left(\mathsf{a}_2(x,x)\right) d^4x\,. \tag{1.133}$$

A similar computation for the operator $\hat{A} = \triangle_{0\mu\nu}$ can easily be performed, giving:

$$\zeta_{\triangle_{0\mu\nu}}(0) = \frac{1}{16\,\pi^2} \int \operatorname{Tr}\left(\mathsf{b}_{2,\mu\nu}(x,x)\right) d^4x\,. \tag{1.134}$$

Here the trace of $\mathsf{b}_{2,\mu\nu}(x,x)$ is over the $SU(N)$ group indices as well as Lorentz indices, i.e.

$$\operatorname{Tr}\left(\mathsf{b}_{2,\mu\nu}(x,x)\right) = \sum_{\mu=0}^{3} \sum_{a=1}^{N^2-1} \mathsf{b}^{aa}_{2,\mu\mu}(x,x)\,. \tag{1.135}$$

Now, the main task is to determine $\mathsf{a}_2(x,x)$ and $\mathsf{b}_{2,\mu\nu}(x,x)$. Substituting the asymptotic expansions (1.125) and (1.126) into the corresponding heat equations (1.123) and equating terms of the same order in t yields the following recurrence relations for $\mathsf{a}_n(x,y)$ and $\mathsf{b}_{n,\mu\nu}(x,y)$:

$$(x-y)_\mu\, \mathfrak{D}_\mu \mathsf{a}_0(x,y) = 0\,, \tag{1.136}$$

$$n\,\mathsf{a}_n(x,y) + (x-y)_\mu\, \mathfrak{D}_\mu \mathsf{a}_n(x,y) = \mathfrak{D}^2\, \mathsf{a}_{n-1}(x,y)\,, \qquad n \geq 1, \tag{1.137}$$

$$(x-y)_\sigma\, \mathfrak{D}_\sigma \mathsf{b}_{0,\mu\nu}(x,y) = 0\,, \tag{1.138}$$

$$n\,\mathsf{b}_{n,\mu\nu}(x,y) + (x-y)_\sigma\, \mathfrak{D}_\sigma \mathsf{b}_{n,\mu\nu}(x,y) = -\triangle_{0\mu\sigma} \mathsf{b}_{n-1,\sigma\nu}(x,y)\,, \quad n \geq 1. \tag{1.139}$$

Repeated applications of $\mathfrak{D}_\mu$ to these equations, followed by setting $x = y$, enables us to solve for $\mathsf{a}_n(x,x)$, $\mathsf{b}_{n,\mu\nu}(x,x)$ and their derivatives. Starting with (1.137) and (1.139) for $n = 1$, we can write:

$$\mathsf{a}_1(x,x) = \mathfrak{D}^2\, \mathsf{a}_0(x,y)\Big|_{x=y}\,, \tag{1.140}$$

$$\mathsf{b}_{1,\mu\nu}(x,x) = \mathfrak{D}^2\, \mathsf{b}_{0,\mu\nu}(x,y)\Big|_{x=y} + 2\, F^{\mathsf{adj}}_{\mu\nu}(x)\,. \tag{1.141}$$

To evaluate $\mathfrak{D}_\lambda\, \mathsf{a}_0$, $\mathfrak{D}^2\, \mathsf{a}_0$, $\mathfrak{D}_\lambda\, \mathsf{b}_{0,\mu\nu}$ and $\mathfrak{D}^2\, \mathsf{b}_{0,\mu\nu}$ at $x = y$, we do the following:

- firstly, we operate on (1.136) and (1.138) with $\mathfrak{D}_\lambda$ and then set $x = y$ to obtain:

$$\mathfrak{D}_\lambda \mathsf{a}_0(x,y)\Big|_{x=y} = \mathfrak{D}_\lambda \mathsf{b}_{0,\mu\nu}(x,y)\Big|_{x=y} = 0\,, \tag{1.142}$$

- secondly, we repeat the first step using $\mathfrak{D}_\lambda\, \mathfrak{D}_\beta$ instead of $\mathfrak{D}_\lambda$ to obtain:

$$(\mathfrak{D}_\lambda \mathfrak{D}_\beta + \mathfrak{D}_\beta \mathfrak{D}_\lambda)\mathsf{a}_0(x,y)\Big|_{x=y} = (\mathfrak{D}_\lambda \mathfrak{D}_\beta + \mathfrak{D}_\beta \mathfrak{D}_\lambda)\mathsf{b}_{0,\mu\nu}(x,y)\Big|_{x=y} = 0\,, \tag{1.143}$$

  which leads to:

$$\mathsf{a}_1(x,x) = 0\,, \qquad \mathsf{b}_{1,\mu\nu}(x,x) = 2\, F^{\mathsf{adj}}_{\mu\nu}(x)\,. \tag{1.144}$$

Also, from (1.137) and (1.139) for $n = 2$ and by use of (1.144) for the value of $\mathsf{b}_{1,\mu\nu}(x,x)$,

it follows that:

$$\mathsf{a}_2(x,x) = \frac{1}{2}\,\mathfrak{D}^2\,\mathsf{a}_1(x,y)\Big|_{x=y}\,, \tag{1.145}$$

$$\mathsf{b}_{2,\mu\nu}(x,x) = \frac{1}{2}\,\mathfrak{D}^2\,\mathsf{b}_{1,\mu\nu}(x,y)\Big|_{x=y} + 2\,F^{\mathsf{adj}}_{\mu\sigma}(x)\,F^{\mathsf{adj}}_{\sigma\nu}(x)\,. \tag{1.146}$$

By applying $\mathfrak{D}^2$ to (1.137) and (1.139) for $n=1$ and then letting $x=y$, we find that:

$$\mathfrak{D}^2\mathsf{a}_1(x,y)\Big|_{x=y} = \frac{1}{3}\,\mathfrak{D}^2\,\mathfrak{D}^2\,\mathsf{a}_0(x,y)\Big|_{x=y}\,, \tag{1.147}$$

$$\mathfrak{D}^2\mathsf{b}_{1,\mu\nu}(x,y)\Big|_{x=y} = \frac{1}{3}\,\mathfrak{D}^2\,\mathfrak{D}^2\mathsf{b}_{0,\mu\nu}(x,y)\Big|_{x=y} + \frac{2}{3}\,\mathfrak{D}^2\left(F^{\mathsf{adj}}_{\mu\sigma}\;\mathsf{b}_{0,\sigma\nu}(x,y)\right)\Big|_{x=y}\,, \tag{1.148}$$

where

$$\begin{aligned}\mathfrak{D}^2\left(F^{\mathsf{adj}}_{\mu\sigma}\;\mathsf{b}_{0,\sigma\nu}(x,y)\right) &= \left(\mathfrak{D}^2F^{\mathsf{adj}}_{\mu\sigma}\right)\mathsf{b}_{0,\sigma\nu}(x,y) + 2\left(\mathfrak{D}_\lambda\,F^{\mathsf{adj}}_{\mu\sigma}\right)\mathfrak{D}_\lambda\mathsf{b}_{0,\sigma\nu}(x,y)\\ &\quad + F^{\mathsf{adj}}_{\mu\sigma}(x)\,\mathfrak{D}^2\,\mathsf{b}_{0,\sigma\nu}(x,y)\,,\end{aligned} \tag{1.149}$$

which at $x=y$ reduces, with the help of (1.142) and (1.143), to:

$$\mathfrak{D}^2\left(F^{\mathsf{adj}}_{\mu\sigma}\;\mathsf{b}_{0,\sigma\nu}(x,y)\right)\Big|_{x=y} = \mathfrak{D}^2F^{\mathsf{adj}}_{\mu\nu}(x)\,. \tag{1.150}$$

So far, only $\mathfrak{D}^2\,\mathfrak{D}^2\,\mathsf{a}_0(x,y)\Big|_{x=y}$ and $\mathfrak{D}^2\,\mathfrak{D}^2\,\mathsf{b}_{0,\mu\nu}(x,y)\Big|_{x=y}$ are left to be determined for the evaluation of $\mathsf{a}_2(x,x)$ and $\mathsf{b}_{2,\mu\nu}(x,x)$. As these can be calculated in a similar way, we shall consider finding $\mathfrak{D}^2\,\mathfrak{D}^2\,\mathsf{a}_0(x,y)\Big|_{x=y}$ only. By applying the operator $\mathfrak{D}_\beta\,\mathfrak{D}_\rho\,\mathfrak{D}_\lambda\,\mathfrak{D}_\upsilon$ to (1.136), from left to right, and then setting $x=y$ we obtain a useful identity:

$$\left(\mathfrak{D}_\beta\,\mathfrak{D}_\rho\,\mathfrak{D}_\lambda\,\mathfrak{D}_\upsilon + \mathfrak{D}_\beta\,\mathfrak{D}_\rho\,\mathfrak{D}_\upsilon\,\mathfrak{D}_\lambda + \mathfrak{D}_\beta\,\mathfrak{D}_\lambda\,\mathfrak{D}_\upsilon\,\mathfrak{D}_\rho + \mathfrak{D}_\rho\,\mathfrak{D}_\lambda\,\mathfrak{D}_\upsilon\,\mathfrak{D}_\beta\right)\mathsf{a}_0(x,y)\Big|_{x=y} = 0, \tag{1.151}$$

from which we deduce the following relations:

$$\mathfrak{D}^2\,\mathfrak{D}^2\,\mathsf{a}_0(x,y)\Big|_{x=y} = -\mathfrak{D}_\mu\,\mathfrak{D}^2\,\mathfrak{D}_\mu\,\mathsf{a}_0(x,y)\Big|_{x=y}\,, \tag{1.152}$$

$$\mathfrak{D}_\mu\,\mathfrak{D}_\nu\,\mathfrak{D}_\mu\,\mathfrak{D}_\nu\,\mathsf{a}_0(x,y)\Big|_{x=y} = \left(\frac{1}{2}\,[\mathfrak{D}_\mu,\mathfrak{D}_\nu]^2 + \mathfrak{D}_\mu\,\mathfrak{D}^2\,\mathfrak{D}_\mu\right)\mathsf{a}_0(x,y)\Big|_{x=y} = 0\,, \tag{1.153}$$

giving:

$$\mathfrak{D}^2\,\mathfrak{D}^2\,\mathsf{a}_0(x,y)\Big|_{x=y} = \frac{1}{2}\,[\mathfrak{D}_\mu,\mathfrak{D}_\nu]^2\,\mathsf{a}_0(x,y)\Big|_{x=y} = \frac{1}{2}\,F^{\mathsf{adj}}_{\mu\nu}(x)\,F^{\mathsf{adj}}_{\mu\nu}(x)\,. \tag{1.154}$$

In a similar way, we can show that:

$$\mathfrak{D}^2\,\mathfrak{D}^2\,\mathsf{b}_{0,\mu\nu}(x,y)\Big|_{x=y} = \frac{1}{2}\,F^{\mathsf{adj}}_{\lambda\beta}(x)\,F^{\mathsf{adj}}_{\lambda\beta}(x)\,\delta_{\mu\nu}\,. \tag{1.155}$$

Finally, we use these results in (1.147) and (1.148) to obtain:

$$\mathsf{a}_2(x,x) = \frac{1}{12}\,F^{\mathsf{adj}}_{\mu\nu}(x)\,F^{\mathsf{adj}}_{\mu\nu}(x)\,, \tag{1.156}$$

$$\mathsf{b}_{2,\mu\nu}(x,x) = \frac{1}{12}\,F^{\mathsf{adj}}_{\lambda\beta}(x)\,F^{\mathsf{adj}}_{\lambda\beta}(x)\,\delta_{\mu\nu} + 2\,F^{\mathsf{adj}}_{\mu\lambda}(x)\,F^{\mathsf{adj}}_{\lambda\nu}(x) + \frac{1}{3}\,\mathfrak{D}^2\,F^{\mathsf{adj}}_{\mu\nu}(x)\,. \tag{1.157}$$

The traces of these quantities over their Lorentz and $SU(N)$ group indices are:

$$\mathrm{Tr}\,(\mathsf{a}_2(x,x)) = -\frac{1}{12}\,N\,F^a_{\mu\nu}(x)\,F^a_{\mu\nu}(x)\,, \tag{1.158}$$

$$\mathrm{Tr}\,(\mathsf{b}_{2,\mu\nu}(x,x)) = \frac{5}{3}\,N\,F^a_{\mu\nu}(x)\,F^a_{\mu\nu}(x)\,. \tag{1.159}$$

Here, the last term in (1.157) does not contribute as it vanishes on taking the trace over Lorentz indices. In calculating the above traces, we have made use of (1.68) and the fact that $\mathrm{Tr}\,(\delta_{\mu\nu}) = 4$.

Substituting (1.158) and (1.159) into (1.133) and (1.134) respectively gives:

$$\zeta_{-\mathfrak{D}^2}(0) = -\frac{N}{12}\,\frac{1}{16\,\pi^2}\int F^a_{\mu\nu}(x)F^a_{\mu\nu}(x)\,d^4x = -\frac{N}{12}\,\frac{1}{4\,\pi^2}\,S_E[B_\mu]\,, \tag{1.160}$$

$$\zeta_{\triangle_{0\mu\nu}}(0) = \frac{5N}{3}\,\frac{1}{16\,\pi^2}\int F^a_{\mu\nu}(x)F^a_{\mu\nu}(x)\,d^4x = \frac{5N}{3}\,\frac{1}{4\,\pi^2}\,S_E[B_\mu]\,. \tag{1.161}$$

These together with the identity of (1.113) allow us to write (1.102) as:

$$\begin{aligned} Z &= C\,\frac{\det\left(-\mathfrak{D}^2\right)}{\det\left(\triangle_{0\,\mu\nu}\right)^{1/2}}\;\mathrm{e}^{-S_E[B_\mu]/g^2}\;\mathrm{e}^{[-\zeta_{-\mathfrak{D}^2}(0)+\zeta_{\triangle_{0\mu\nu}}(0)/2]\ln q^2} \\ &= C'\,\exp\left(-\Big(\frac{4\pi}{g^2} - \frac{11}{3}\,\frac{N}{4\pi}\,\ln q^2\Big)S_E[B_\mu]/\pi\right)\,. \end{aligned} \tag{1.162}$$

Here, we have lumped C and $\det(-\mathfrak{D}^2)/\det(\triangle_{0\,\mu\nu})^{1/2}$ in C' because they are both constants

independent of q^2 and g. Since Z is not supposed to depend on the mass scale parameter q, which was introduced arbitrarily, we tune the coupling constant g such that:

$$\frac{4\pi}{g^2} - \frac{11}{3}\frac{N}{4\pi}\ln q^2 = \text{constant} \equiv \frac{11}{3}\frac{N}{4\pi}\ln \Lambda^2 , \tag{1.163}$$

giving:

$$g^2 = \frac{(4\pi)^2}{11N/3}\ \frac{1}{\ln(q^2/\Lambda^2)} , \tag{1.164}$$

where Λ is a fixed-reference scale with dimension of mass. In this way, the arbitrary mass scale q in (1.162) is removed in favour of Λ, redefining g as a scale dependent quantity.

In QCD, we have $N = 3$, i.e. the number of colour charges. Therefore, we can easily determine from (1.164) the effective QCD coupling constant $\alpha_{\rm PT}^{(1)} = g^2/4\pi$, giving:

$$\alpha_{\rm PT}^{(1)}(Q^2) = \frac{4\pi}{\beta_0}\frac{1}{\ln(Q^2/\Lambda^2)} , \qquad \text{with} \qquad \beta_0 = 11 . \tag{1.165}$$

Here, for consistency with the standard definition in QCD literature, we have identified q^2 with the momentum-transfer squared Q^2 which defines the scale of the physics that we are probing. Had we included the quark fields in our calculation, we would have obtained the same expression as in (1.165) for the effective QCD coupling except for the β_0-factor which would then be [12]:

$$\beta_0 = 11 - \frac{2}{3}n_f , \tag{1.166}$$

where n_f denotes the number of quark flavours.

For $\beta_0 > 0$, which is the case if $0 \leq n_f \leq 16$, we can easily deduce from (1.165) that the coupling constant decreases with increasing Q^2 and approaches zero at infinitely large Q^2. This implies that the energy of the interaction between quarks decreases as their separation decreases, which contrasts with the case of electric charges whose interaction energy grows when they approach each other. In other words, quarks within a hadron behave as essentially free particles. This property is known as the asymptotic freedom [12].

1.3 Causal analyticity, physical observables and our goals

A fundamental problem in the theory of particle physics lies in the description of hadron interactions in the infrared region. The property of asymptotic freedom in QCD allows us

to investigate the interactions of quarks and gluons at short distances using the standard perturbation theory. However, there is a number of phenomena whose description is intractable in perturbation theory, for example quark confinement and gluon and quark condensates. Hence, the search for calculational techniques that go beyond conventional perturbation theory remains essential (not only in QCD but in other field theories as well).

In standard perturbative QCD, the running coupling constant diverges at a small mass scale $Q = \Lambda$, creating the so-called Landau ghost-pole problem. Taking next loop corrections into account does not alter the essence, and leads only to additional branch cuts along the real axis $\mathrm{Re}\{Q^2\} > 0$. This problem prevents the use of perturbative expansion at small momentum transfers $Q \sim \Lambda$ and, in addition, generates infrared (IR) renormalon singularities on the positive real axis of the Borel parameter, destroying attempts to sum up the perturbative series [13–16]. Generally speaking, as Q^2 comes below or near Λ^2, non-perturbative effects become the most dominant and the perturbative expansion becomes useless.

Another indication that the perturbative formalism is incomplete, and cannot describe the low energy physics unless it is supplemented by non-perturbative corrections, comes from considering its analyticity structure in the complex Q^2-plane [17]; the upshot being that any QCD observable, which depends on a spacelike [6] momentum variable Q^2, is expected to be an analytic function of Q^2 in the entire complex plane except the negative real (timelike) axis. Singularities on the timelike axis are meaningful since they correspond to production of on-shell particles, while their existence on the spacelike axis is non-physical as this would violate causality (i.e. causal analyticity structure) [17, 18]. For example, if a generic QCD observable were calculated to leading order, it would depend on $\alpha_{\mathrm{PT}}^{(1)}(Q^2)$, inheriting the Landau-singularity at $Q^2 = \Lambda^2$. This singularity is obviously non-physical as it lies on the positive real axis $\mathrm{Re}\{Q^2\} > 0$. From this point of view, causality constrains the Q^2-dependence of physical observables, and is consistent with perturbative results only if the coupling constant is non-singular on the entire Q^2-plane with the exception of the timelike axis $\mathrm{Re}\{Q^2\} < 0$.

A small number of models for the QCD running coupling $\alpha(Q^2)$ have been proposed

[6] Following [19], the metric with signature (-1,1,1,1) is used from now on so that $Q^2 > 0$ corresponds to a spacelike (Euclidean) 4-momentum transfer.

[16, 18–21] to comply with the causality condition, i.e. the requirement of analyticity in Q^2. However, the issue of which of these is the most realistic is still a moot point. Quite recently, a good attempt has been made, by Shirkov and Solovtsov [19], to devise a model for the running coupling that is completely free of singularities in the IR region. In this approach, the analytic running coupling is defined via the so-called Källén-Lehmann spectral representation as:

$$\alpha_{\rm an}^{(n)}(Q^2) = 4\int_0^\infty \frac{\rho^{(n)}(x)}{(x+Q^2-i\,0)}\,dx\,, \tag{1.167}$$

with the n-loop spectral density $\rho^{(n)}(x)$ given by:

$$\rho^{(n)}(x) = \frac{1}{4\pi}{\rm Im}\{\alpha_{\rm PT}^{(n)}(-x-i\,0)\}\,, \tag{1.168}$$

where $\alpha_{\rm PT}^{(n)}$ is the coupling constant obtained from perturbation theory (PT) at the n-loop approximation. To leading order, the corresponding spectral density reads as:

$$\rho^{(1)}(x) = \frac{\pi}{\beta_0}\,\frac{1}{[\pi^2+\ln^2(x/\Lambda^2)]}\,. \tag{1.169}$$

Inserting this into (1.167) gives the one-loop analytic spacelike coupling constant:

$$\alpha_{\rm an}^{(1)}(Q^2) = \frac{4\pi}{\beta_0}\left[\frac{1}{\ln(Q^2/\Lambda^2)} + \frac{1}{1-Q^2/\Lambda^2}\right]. \tag{1.170}$$

This expression is consistent with the causality condition. The first term on the right-hand side of (1.170) preserves the standard ultraviolet (UV) behaviour whereas the second term compensates for the ghost-pole at $Q^2=\Lambda^2$. Obviously the second term in (1.170) comes from the spectral representation and enforces the required analytic properties. Thus, it is essentially non-perturbative. However, as mentioned in Ref. [18], as this term introduces a $1/Q^2$ correction to $\alpha_{\rm PT}^{(1)}(Q^2)$ at large Q^2 it would make (1.170) unsuitable as an input quantity for observables that are proportional to the running coupling (in leading order) but are not expected to have $1/Q^2$ corrections (such as the e^+e^- total cross section) because in such cases the unwanted $1/Q^2$ correction would have to be artificially cancelled.

By construction, (1.170) does not include any adjustable parameters other than the QCD characteristic mass scale Λ. Thus, one might prefer to have a model with free extra

parameters that would allow for the fitting of the coupling to lower energy experimental data and hence further improve perturbative results at low Q^2. An example of a model of this type is suggested in Ref. [20], where the one-loop coupling constant assumes the form:

$$\alpha^{(1)}(Q^2) = \frac{4\pi}{\beta_0}\left[\frac{Q^{2p}/\Lambda^{2p}}{Q^{2p}/\Lambda^{2p}+C_p}\right]\frac{p}{\ln(Q^{2p}/\Lambda^{2p}+C_p)}, \tag{1.171}$$

with $C_p \geq 1$. For $Q^2 \gg \sqrt[p]{C_p}\,\Lambda^2$, this expression recovers the perturbative asymptotic form (1.165). Although (1.171) is a ghost-pole free expression, being analytic for all $Q^2 \in [0,\infty)$, it contains unphysical singularities on the complex Q^2-plane (for all $p > 1$) and hence does not comply with causality.

A careful analytic study of non-perturbative effects is always important in QCD because it provides more reliable and useful information about the IR region, which is inaccessible to perturbative methods. The main purpose of this thesis is to construct a new analytic approach based on a different and more general methodology to that of Shirkov and Solovtsov, which improves perturbative results outside the asymptotic domain and respects the causal analyticity structure in, at least, the right half of the complex Q^2-plane. Having achieved this, we apply our method to the QCD coupling constant to solve the Landau ghost-pole problem without altering the correct perturbative behaviour in the UV region. Then, we show that the resultant QCD coupling in this way freezes to a finite value at the origin (i.e. $Q^2 = 0$), supporting the IR freezing idea which has long been a popular and successful phenomenological hypothesis [22,24]. Moreover, from the viewpoint of the new background field formalism [14,15] our approach provides better estimates for the IR fixed points than that of Shirkov and Solovtso.

The layout of this thesis is as follows: In chapter 2, we discuss our analyticization procedure on general grounds, proposing a new integral representation for physical observables that depend on a spacelike momentum variable (squared) Q^2. In this chapter, we present a full derivation of our coupling constant $\bar{\alpha}^{(1)}(Q^2)$, giving a new expression that depends on a free extra parameter λ_e which can be used to tune the coupling to lower energy experimental data. An approximation scheme for estimating the value of λ_e is included in section 2.3. In chapter 3, we carry out a comprehensive comparison between the predictions in our approach and those estimated by other theoretical methods, which include conventional perturbation theory, optimized perturbation theory, background field

formalism and the analytic approach of Shirkov and Solovtsov. In section 3.3, we test our model on a fit-invariant IR characteristic integral extracted from jet physics data. In section 3.6, we use our analytic coupling constant in the instanton density derived from the dilute instanton-gas approximation to estimate the gluon condensate. Then, we show that the result obtained is in good agreement with the value phenomenologically estimated from the QCD sum rules. In section 3.7, we calculate the $\beta-$function which corresponds to our analytic coupling constant and compare its behaviour with the perturbative counterpart. We further show that the the $\beta-$function in our approach and that in higher-loop order perturbation theory behave qualitatively the same in the range of n_f-values that allows perturbation theory to obtain IR fixed points. In chapter 4, we extend our calculations to include the exact two-loop perturbative expression of the coupling constant $\bar{\alpha}^{(2)}_{LW}(q)$, where $q = Q^2/\Lambda^2$. For the set up of this computation, we give a detailed study of the singularity structure of $\bar{\alpha}^{(2)}_{LW}(q)$ which is essential for the analytic continuation of $\bar{\alpha}^{(2)}_{LW}(q)$ to the complex q-plane as required in our method. In this chapter, we show how to remove the unphysical cut together with the Landau ghost-pole singularity from the perturbative expression $\bar{\alpha}^{(2)}_{LW}(q)$ without altering the correct UV properties including asymptotic freedom. Plots describing the IR and UV behaviour of the coupling constant in our approach and the new background field formalism at the two-loop level are illustrated in section 4.6. Our relatively low energy prediction, unlike the new background field formalism, turns out to be in good agreement with that obtained from the fits to charmonium spectrum and fine structure splitting in Ref [37].

In chapter 5, we give a detailed study of the Schrödinger representation in quantum field theory (QFT), presenting a further application of our approach in the area of wave functionals. In this chapter, we show that for an interacting scalar field theory with a non-zero mass gap the Schrödinger vacuum functional $\Psi_0[\varphi]$ undergoes a significant simplification when evaluated for fields $\varphi(x)$ whose Fourier transforms $\widetilde{\varphi}(k)$ have sufficiently small supports. As we will show this is because its logarithm $\mathsf{W}_0[\varphi]$ reduces to a local functional expansion, i.e. a single spatial integral of a sum of terms each composed of $\varphi(x)$ and/or a finite number of its derivatives at the same spatial point. A knowledge of this expansion or its leading terms enables us to estimate the vacuum $\Psi_0[\varphi] = \exp\big(\mathsf{W}_0[\varphi]\big)$ for an arbitrary source field by exploiting the analyticity of $\mathsf{W}_0[\varphi_s]$ in a complex scale parameter s, where $\varphi_s = \varphi(x/\sqrt{s})$. By studying the analyticity of W_0 for the scaled field

φ_s, we find that it extends to an analytic function of s on the whole of the complex s-plane with a branch cut restricted to the negative real axis. This property of analyticity in the complex s-plane is the basis of our method because it allows the use of Cauchy's theorem for relating the large-s behaviour, where the local expansion of $\mathsf{W}_0[\varphi_s]$ holds, to the point $s = 1$.

In appendix A, we carry out some of the contour integrations involved in our computation. In appendix B, we illustrate a useful method for solving inhomogeneous differential equations subject to Dirichlet boundary conditions, using Green's functions. The last chapter is devoted to our conclusions.

Chapter 2

An Analytic Approach to Physical Observables

2.1 Analyticization Procedure

We will illustrate our method with the following pedagogical example. Consider a physical observable F depending on a positive variable q with the dimensions of energy squared. Then, it follows from the principle of causality, mentioned earlier, that $F(q)$ can be analytically continued to the complex plane excluding the negative real axis. As we shall show, this will allow us to reconstruct $F(q)$ from its high energy behaviour by using the contour integral representation:

$$\bar{F}(q,\lambda) = \frac{1}{2\pi i}\int_{C_{UV}} \frac{e^{\lambda(k-q)}}{k-q}\, F(k)\, dk\,, \tag{2.1}$$

where C_{UV} is a very large incomplete circle, in the complex $k-$plane, with radius R_{UV} and centre at the origin, beginning just below the negative real axis and ending just above and $q \in \{\ \mathrm{Re}\ k\ :\ 0 < \mathrm{Re}\ k < R_{UV}\}$ as depicted in Fig.(2.1).

We will show that $F(q)$ is recovered as the limit as $\lambda \to \infty$ of $\bar{F}(q,\lambda)$, and this depends mainly on the ultraviolet behaviour of $F(q)$ when we take R_{UV} to be sufficiently large. In order to achieve this goal, we exploit the analyticity of $F(k)$ in the complex k-plane, using Cauchy's theorem to replace the UV-boundary C_{UV} in (2.1) with a small circle C_0 around q and a keyhole shaped contour C_k, depicted in Fig.(2.2), surrounding the cut and not connected to C_0. For this deformed contour, Cauchy's integral formula over the circle

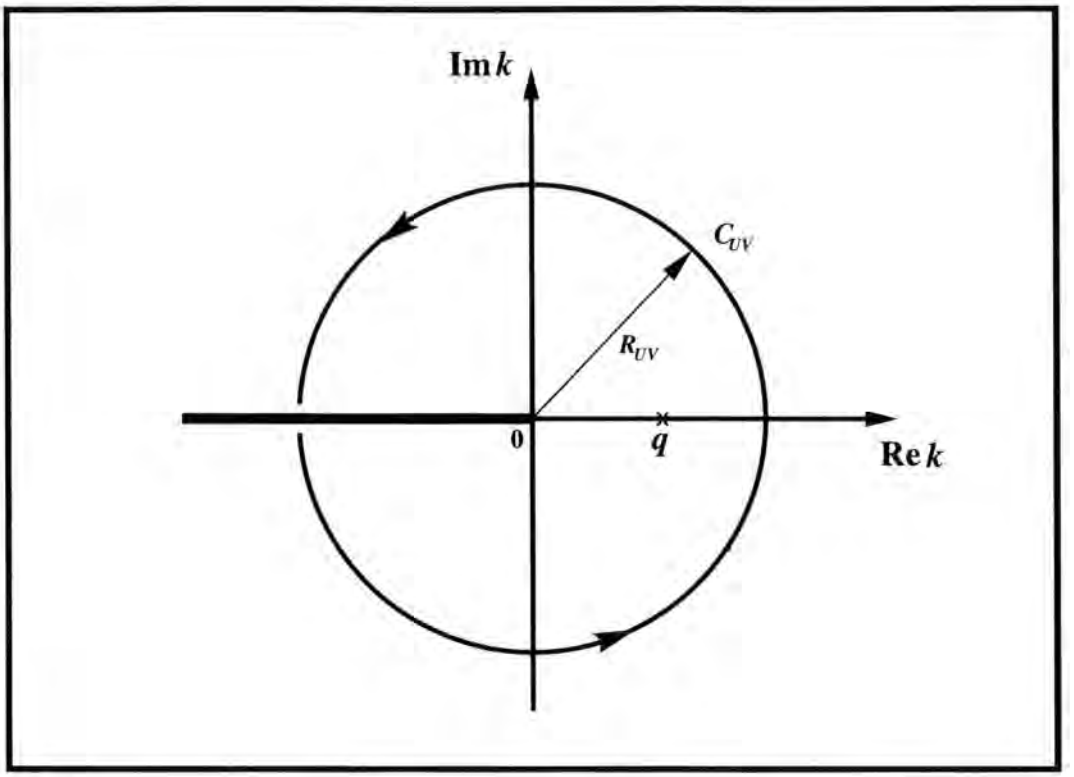


Figure 2.1: Sketch of the integration contour C_{UV} in the cut complex $k-$plane. The thick line represents a branch cut and the cross indicates the location of q.

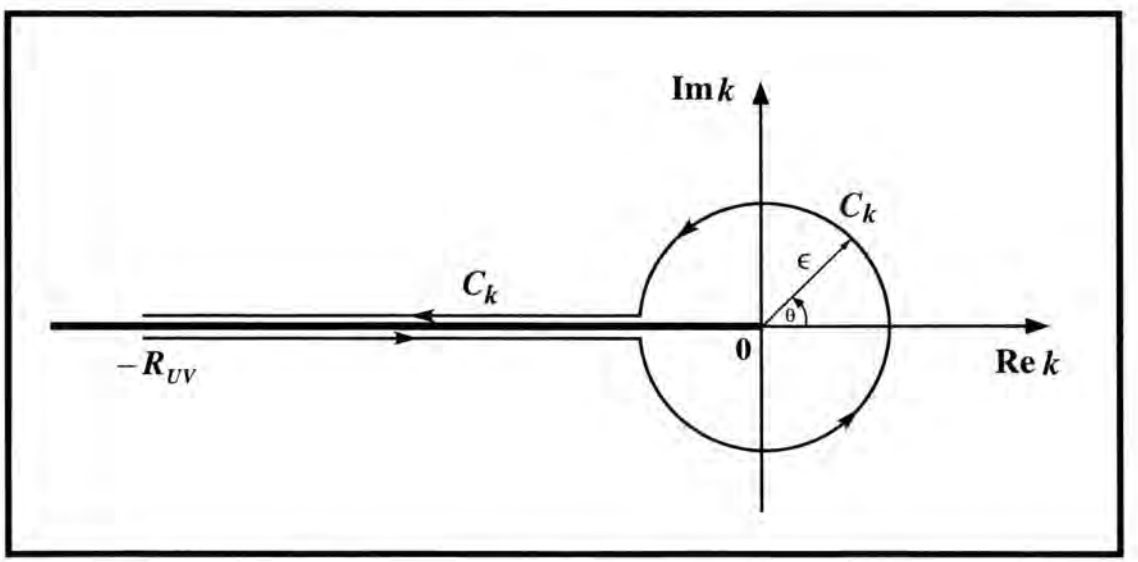


Figure 2.2: Sketch of the keyhole shaped contour C_k. The thick line represents the branch cut Re $k \leq 0$.

C_0 yields $F(q)$ which together with the integral over the keyhole contour C_k transforms the integral (2.1) into the form:

$$\bar{F}(q,\lambda) = F(q) + I_{C_k}\,, \tag{2.2}$$

where

$$I_{C_k} = \frac{1}{2\pi i}\int_{C_k} \frac{\mathrm{e}^{\lambda(k-q)}}{k-q}\, F(k)\, dk\,. \tag{2.3}$$

If we restrict attention to those functions $F(k)$ which are finite on the line of discontinuity along the negative real k-axis, e.g. $F(k) \propto \sqrt{k}$, then we can write I_{C_k} more explicitly as:

$$I_{C_k} = \int_{\epsilon}^{R_{UV}} \frac{\mathrm{e}^{-\lambda(r+q)}}{r+q}\, \Delta(r)\, dr + \frac{\epsilon\, \mathrm{e}^{-\lambda q}}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{\lambda\epsilon\cos(\theta)}\, \mathrm{f}_\epsilon(\theta,q)\, d\theta, \tag{2.4}$$

with

$$\Delta(r) = \frac{1}{2\pi i}\left[\, F(r\,\mathrm{e}^{i\pi}) - F(r\,\mathrm{e}^{-i\pi})\,\right], \tag{2.5}$$

and

$$\mathrm{f}_\epsilon(\theta,q) = \frac{1}{2}\left[\frac{\mathrm{e}^{i\lambda\epsilon\sin(\theta)}\, F(\epsilon \mathrm{e}^{i\theta})}{\epsilon - q\,\mathrm{e}^{-i\theta}} + \frac{\mathrm{e}^{-i\lambda\epsilon\sin(\theta)}\, F(\epsilon \mathrm{e}^{-i\theta})}{\epsilon - q\,\mathrm{e}^{i\theta}}\right]. \tag{2.6}$$

Owing to the discontinuity of $F(k)$ across the cut, given by $2\pi i\Delta(|k|)$, the sum of the line integrals on each side of the branch cut does not cancel. Since the region of analyticity of $F(k)$:

$$S_{an} = \{k = r\,\mathrm{e}^{i\theta} : r > 0\,,\ -\pi < \theta \leq \pi\}, \tag{2.7}$$

includes a portion of the real axis on which $F(k)$ is real, it follows that $F(k)$ satisfies the Schwarz Reflection Principle [27]:

$$F^*(k) = F(k^*). \tag{2.8}$$

This allows us to rewrite $\Delta(r)$ and $\mathrm{f}_\epsilon(\theta)$ in the more compact forms:

$$\Delta(r) = \frac{1}{\pi}\,\mathrm{Im}\Big\{\, F(r\,\mathrm{e}^{i\pi})\,\Big\}, \tag{2.9}$$

and

$$\mathrm{f}_\epsilon(\theta,q) = \mathrm{Re}\left\{\frac{\mathrm{e}^{i\lambda\epsilon\sin(\theta)}\, F(\epsilon\,\mathrm{e}^{i\theta})}{\epsilon - q\,\mathrm{e}^{-i\theta}}\right\}, \tag{2.10}$$

which imply that I_{C_k} is a purely real quantity as it should be.

In the following, we will investigate the behaviour of I_{C_k} at sufficiently large values of λ. Since $F(r\,e^{i\theta})$ is assumed finite throughout the whole region S_{an}, we take its magnitude to be bounded on the infinitesimal circle $|k| = \epsilon$, see Fig.(2.2), such that:

$$|F(\epsilon\, e^{i\theta})| \leq M\,, \qquad \text{for} \quad -\pi < \theta \leq \pi\,, \tag{2.11}$$

where M is a positive constant which may depend on ϵ. Using this to estimate the upper bound of the second term in (2.4), we find that:

$$\frac{\epsilon\, e^{-\lambda q}}{2\pi}\left|\int_{-\pi}^{\pi} e^{\lambda\epsilon\cos(\theta)}\ f_\epsilon(\theta,q)\ d\theta\right| \leq \frac{\epsilon\, M\, e^{-\lambda(q-\epsilon)}}{q-\epsilon}. \tag{2.12}$$

If we consider only those functions F for which M can be chosen such that $\lim_{\epsilon\to 0}\epsilon M = 0$ then the second term in (2.4) will vanish in this limit and accordingly I_{C_k} reduces to the form:

$$I_{C_k}(q,\lambda) = \int_0^{R_{UV}} \frac{e^{-\lambda(r+q)}}{r+q}\ \Delta(r)\ dr, \qquad q > 0\,, \tag{2.13}$$

which is more suitable for further calculations. For the case under consideration, since $\Delta(r)$ has an upper bound $N > 0$, i.e. $|\Delta(r)| \leq N$, in the interval $0 \leq r \leq R_{UV}$, we deduce that:

$$|I_{C_k}| \leq N\,\frac{e^{-\lambda q}}{\lambda q}\left(1 - e^{-\lambda R_{UV}}\right). \tag{2.14}$$

So for large values of λ, the function $I_{C_k}(q,\lambda)$ decays rapidly to zero, and:

$$\lim_{\lambda\to\infty} I_{C_k}(q,\lambda) = 0\,. \tag{2.15}$$

In general, (2.15) remains true even if the finiteness restriction on $F(k)$ along the negative real k-axis, together with the constraint $\lim_{\epsilon\to 0}\epsilon M = 0$, is not fulfilled. For example, if $F(k)$ has a finite number of singularities on the negative real axis then we can avoid these points by keeping the two edges of the keyhole contour C_k a small distance δ away from the cut which they surround. In this way, we can rewrite (2.3) as:

$$I_{C_k} = \int_{\epsilon'}^{R_{UV}} e^{-\lambda(x+q)}\ g(x,q,\lambda)\,dx\ +\ \frac{\epsilon\, e^{-\lambda q}}{2\pi}\int_{-\pi+\eta}^{\pi-\eta} e^{\lambda\epsilon\cos(\theta)}\ f_\epsilon(\theta,q)\ d\theta, \tag{2.16}$$

where $\epsilon' = \sqrt{\epsilon^2 - \delta^2}$ with $\epsilon > \delta$, $\eta = \arctan(\delta/\epsilon')$ and:

$$g(x,q,\lambda) = \frac{1}{\pi}\,\mathrm{Im}\left\{\frac{e^{i\lambda\,\delta}}{x+q-i\delta}\;F(-x+i\delta)\right\}. \tag{2.17}$$

Since F is bounded on the contour C_k, we have:

$$|I_{C_k}| \leq \frac{N'}{\pi}\,\frac{e^{-\lambda q}}{\lambda(q+\epsilon'-\delta)}\left[e^{-\lambda\epsilon'} - e^{-\lambda R_{UV}}\right] + \frac{\epsilon\,M\,(\pi-\eta)}{\pi}\;\frac{e^{-\lambda(q-\epsilon)}}{q-\epsilon}, \tag{2.18}$$

where N' is the upper bound of $F(-x+i\delta)$ for all $x \in [\epsilon', R_{UV}]$. As both N' and M are λ-independent, in the limit as $\lambda \to \infty$ we obtain (2.15) as claimed above. So, by taking the limit as $\lambda \to \infty$ in (2.2) we deduce from (2.15) that

$$\lim_{\lambda\to\infty} \bar{F}(q,\lambda) = F(q). \tag{2.19}$$

To have some notion of the functional dependence of $\bar{F}(q,\lambda)$ on λ, for a fixed $q > 0$, consider a simple example where the imaginary part of $F(k)$ assumes a constant value μ_0 along the upper edge of the cut, e.g. $F(k) \propto \ln k$. In this case, we have $\Delta(r) = \mu_0/\pi$ and a straightforward integration of (2.13) yields:

$$I_{C_k}(q,\lambda) = \frac{\mu_0}{\pi}\left[E_1(\lambda q) - E_1(\lambda(q+R_{UV}))\right], \tag{2.20}$$

where $E_1(x)$ denotes the exponential integral function [28] defined by:

$$E_1(x) = \int_x^\infty \frac{e^{-t}}{t}\,dt = -\gamma_{\mathrm{E}} - \ln(x) - \sum_{n=1}^{\infty}\frac{(-1)^n}{n!\,n}\,x^n \qquad \text{for } x > 0. \tag{2.21}$$

Here $\gamma_{\mathrm{E}} \cong 0.577215$ is the well-known Euler's constant. By inserting (2.20) into (2.2) and sending $R_{UV} \to \infty$, we immediately arrive at an explicit solution:

$$\bar{F}(q,\lambda) = F(q) + \frac{\mu_0}{\pi}\,E_1(\lambda q). \tag{2.22}$$

As illustrated by the graph in Fig.(2.3), the variation of $\bar{F}(q,\lambda)$ with respect to λ depends largely on both the sign of μ_0 and the behaviour of $E_1(\lambda q)$. With increasing λ, we see that $\bar{F}(q,\lambda)$ evolves from $-\infty$, for $\mu_0 < 0$, or $+\infty$, for $\mu_0 > 0$, in a continuous progression until it settles down to the value $F(q)$ at large values of λ. Moreover, we discover from

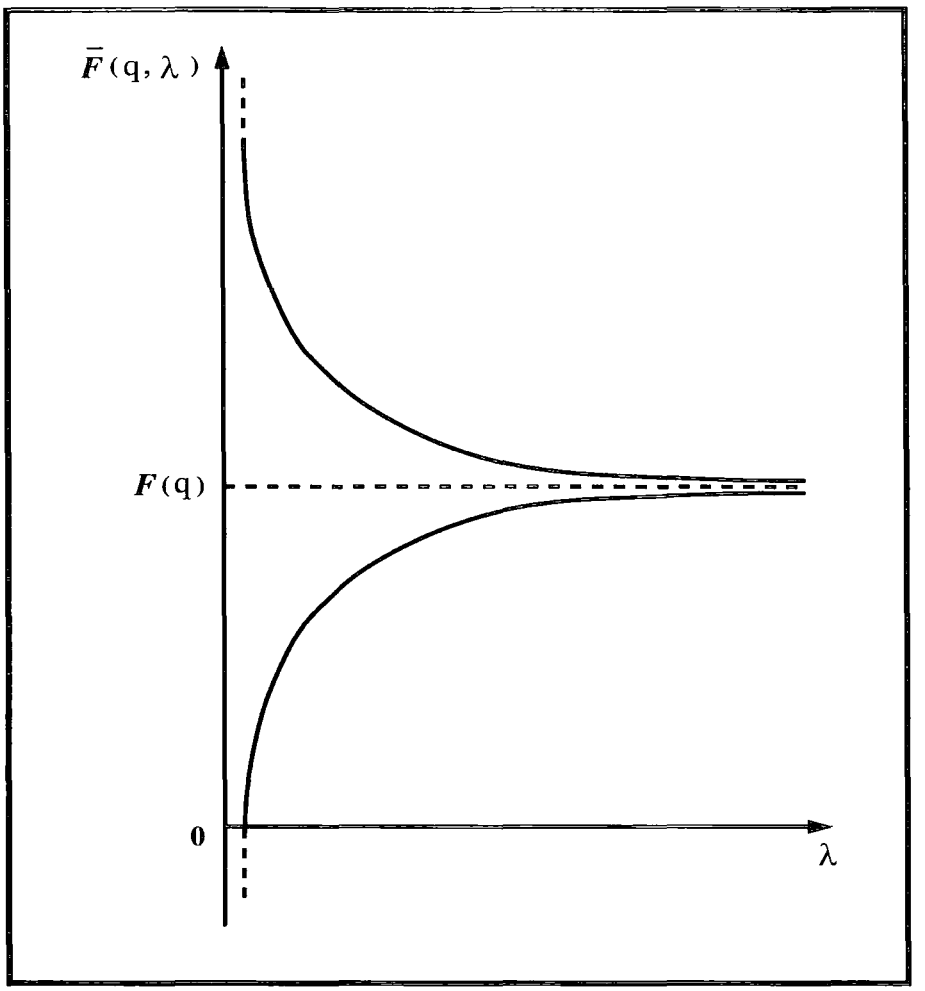


Figure 2.3: The variation of $\bar{F}(q,\lambda)$ versus λ at a fixed value q. The lower and the upper curves describe the cases in which $\mu_0 < 0$ and $\mu_0 > 0$, respectively. The dashed line represents $F(q)$.

(2.22) that $\bar{F}(q,\lambda)$ converges to $F(q)$ faster as q increases.

To summarise, by exploiting the analyticity of $F(k)$ in (2.1), we can obtain $F(q)$ as $\lim_{\lambda\to\infty}\bar{F}(q,\lambda)$, and if we take the radius R_{UV} of the contour C_{UV} to be sufficiently large the integrand depends on the large q behaviour of F. So far, our consideration has been restricted to the case in which $F(q)$, as a true function for the observable in question, complies with the principle of causality. In practice, however, we do not know the function $F(q)$ exactly, even for large q, but for a theory with asymptotic freedom we can approximate the large q behaviour of $F(q)$ using perturbation theory for q in some high energy domain D_{PT} so that $F_{PT}(q) \cong F(q)$ for $q \in D_{PT}$. Thus, for large enough R_{UV}, we can safely use $F_{PT}(k)$ as a reasonable substitute for $F(k)$ in our contour integral (2.1),

where now k is any point on C_{UV}. This gives the approximation $\bar{F}_{PT}(q,\lambda) \approx \bar{F}(q,\lambda)$, but taking λ to infinity in this would simply reproduce the perturbative estimate for $F(q)$, leading to nothing new. Now $F_{PT}(q)$, as a perturbatively calculated quantity, often suffers from a serious defect by having singularities in the complex plane away from the negative real axis. Good examples of this are the effective coupling constant and the running mass in perturbative QCD. These extra singularities are unphysical and do not exist in the true function $F(q)$. Hence, they should be eliminated in our approximation in order to reinstate causality. So, if instead of using the limiting value of $\bar{F}_{PT}(q,\lambda)$ we were to use a finite value of λ, say λ_0, then we might have an expression in which these unphysical singularities are absent and we will give an example in which this happens. Furthermore, taking a finite value of λ in $\bar{F}_{PT}(q,\lambda)$ can give an improvement over the perturbative estimate in favourable circumstances for the following reason: Viewed as a function of λ with q held fixed, $\bar{F}_{PT}(q,\lambda)$ is a better estimate of the true function $\bar{F}(q,\lambda)$ for small λ than it is for large λ since if we scale the integration variable in (2.1) then:

$$\bar{F}_{PT}(q,\lambda) = \frac{1}{2\pi i}\int_{|k|=\lambda R_{UV}} \frac{\mathrm{e}^{k-\lambda q}}{k-\lambda q}\, F_{PT}(k/\lambda)\, dk\,. \tag{2.23}$$

For large enough R_{UV} we can replace the contour of integration in (2.23) by $|k| = R_{UV}$ since the difference this makes is a small contribution from the negative real axis:

$$\delta_0 = \frac{1}{\pi}\left| \int_{\lambda R_{UV}}^{R_{UV}} \frac{\mathrm{e}^{-(k+\lambda q)}}{k+\lambda q}\, \mathrm{Im}\Big\{ F_{PT}(k\,\mathrm{e}^{i\pi}/\lambda) \Big\}\, dk \right|, \tag{2.24}$$

which is exponentially damped. Now we can see that the smaller the value of λ is the larger is the argument of F_{PT} in the integrand of (2.23), and for an asymptotically free theory this gives a better approximation to $\bar{F}(q,\lambda)$. So, $\bar{F}_{PT}(q,\lambda)$ interpolates between the true quantity $\bar{F}(q,\lambda)$ at small λ and the perturbative estimate $F_{PT}(q)$ at large λ. Under favourable circumstances λ can be chosen sufficiently small that $\bar{F}_{PT}(q,\lambda)$ provides a good enough approximation to the exact function $\bar{F}(q,\lambda)$, and sufficiently large that we are estimating the large λ behaviour of the latter, i.e. $F(q)$.

We will now discuss how to choose an appropriate value $\lambda = \lambda_0$ for $\bar{F}_{PT}(q,\lambda)$, depending on the behaviour of F_{PT}, and pinpoint the most favourable situations in which $\bar{F}_{PT}(q,\lambda_0)$ gives a better estimate for $F(q)$ than $F_{PT}(q)$ does. An illustrative example is

perhaps the best way to convey these ideas. Consider the simple case in which $F_{PT}(q)$ suffers only from one infrared singularity at $q = \Lambda^2$ of the simple pole type:

$$F_{PT}(q) = \frac{U(q)}{q - \Lambda^2}\,, \tag{2.25}$$

where $U(q)$ is an analytic function of q in the entire complex $q-$plane excluding the negative real axis (e.g. the principle value of log). Then, define the UV region where the perturbation theory of this toy model is trustworthy by:

$$D_{PT} = \{q : q \gg \Lambda^2\}\,. \tag{2.26}$$

Replacing F and $\bar{F}$ with F_{PT} and $\bar{F}_{PT}$, respectively, in our integral formula (2.1) and then integrating in the usual way, we obtain:

$$\bar{F}_{PT}(q,\lambda) = F_{PT}(q) - \frac{U(\Lambda^2)}{q - \Lambda^2}\,\mathrm{e}^{-\lambda(q-\Lambda^2)} + H(q,\lambda) \qquad \text{for } q \neq \Lambda^2\,, \tag{2.27}$$

and

$$\bar{F}_{PT}(\Lambda^2,\lambda) = \lambda\, U(\Lambda^2) + U'(\Lambda^2) + H(\Lambda^2,\lambda) \qquad \text{for } q = \Lambda^2\,, \tag{2.28}$$

where

$$H(q,\lambda) = \int_0^{R_{UV}} \frac{\mathrm{e}^{-\lambda(r+q)}}{r+q}\,\Delta_{PT}(r)\,dr\,, \qquad q > 0\,, \tag{2.29}$$

with

$$\Delta_{PT}(r) = -\frac{1}{\pi}\,\frac{\mathrm{Im}\{\,U(r\,\mathrm{e}^{i\pi})\,\}}{r + \Lambda^2}\,. \tag{2.30}$$

Here, we have $R_{UV} \gg \Lambda^2$. In this model, (2.27) allows us to modify the perturbative expression $F_{PT}(q)$ through the variable λ. Taking λ to infinity in (2.27) would only reproduce $F_{PT}(q)$:

$$\lim_{\lambda\to\infty} \bar{F}_{PT}(q,\lambda) = F_{PT}(q)\,, \tag{2.31}$$

on the other hand, keeping λ fixed at a finite value λ_0 would change the behaviour of $F_{PT}(q)$, especially in the vicinity of Λ^2, by an infrared correction term:

$$\Upsilon_{IR}(q,\lambda_0) = -\frac{U(\Lambda^2)}{(q - \Lambda^2)}\,\mathrm{e}^{-\lambda_0(q-\Lambda^2)} + H(q,\lambda_0)\,, \tag{2.32}$$

which would, in turn, remove the IR singularity in $F_{PT}(q)$. So, to reinstate the causal analyticity structure violated by the presence of the simple pole singularity on the positive real axis, we would simply retain $\Upsilon_{IR}(q,\lambda_0)$ in our formulation. Note that the continuity of $\bar{F}_{PT}(q,\lambda)$ at $q=\Lambda^2$ for a fixed λ:

$$\lim_{q\to\Lambda^2} \bar{F}_{PT}(q,\lambda) = \bar{F}_{PT}(\Lambda^2,\lambda)\,, \tag{2.33}$$

follows directly from (2.27) and (2.28).

Now, we shall study this example further by investigating the possibility of finding a proper value $\lambda=\lambda_0$ that would allow $\bar{F}_{PT}(q,\lambda_0)$ to match the exact value of the observable $F(q)$ at the point q in question. At the same time, we shall consider the case in which this is not possible and show how to make the best choice of λ_0 that can improve perturbative predictions. To explore straightforwardly the criterion of selecting λ_0, at a fixed value of q, we shall simplify our example further by assuming that $\mathrm{Im}\{U(r\,\mathrm{e}^{i\pi})\}=\omega$, with ω being some real constant. In this case, a straightforward calculation of (2.29) yields:

$$H(q,\lambda) = -\frac{\omega}{\pi(q-\Lambda^2)}\Big\{\mathrm{e}^{-\lambda(q-\Lambda^2)}\Big[\,E_1(\lambda\Lambda^2) - E_1(\lambda(\Lambda^2+R_{UV}))\,\Big] \\ - E_1(\lambda q) + E_1(\lambda(q+R_{UV}))\Big\} \qquad \text{for } q\neq\Lambda^2\,, \tag{2.34}$$

and

$$H(\Lambda^2,\lambda) = -\frac{\omega}{\pi}\,\mathrm{e}^{-\lambda\Lambda^2}\Big\{\frac{1}{\Lambda^2} - \frac{\mathrm{e}^{-\lambda R_{UV}}}{\Lambda^2+R_{UV}} - \lambda\,\mathrm{e}^{\lambda\Lambda^2}\Big[E_1(\lambda\Lambda^2) \\ - E_1(\lambda(\Lambda^2+R_{UV}))\Big]\Big\} \qquad \text{for } q=\Lambda^2\,. \tag{2.35}$$

Note that in the limit as $q\to\Lambda^2$ equation (2.34) tends to (2.35). Substituting (2.34) into (2.27) and then letting $R_{UV}\to\infty$, we obtain:

$$\bar{F}_{PT}(q,\lambda) = F_{PT}(q) - \Big[U(\Lambda^2) + \frac{\omega}{\pi}E_1(\lambda\Lambda^2) - \frac{\omega}{\pi}E_1(\lambda q)\,\mathrm{e}^{\lambda(q-\Lambda^2)}\Big]\frac{\mathrm{e}^{-\lambda(q-\Lambda^2)}}{q-\Lambda^2}\,, \tag{2.36}$$

which together with the first and the second derivatives:

$$\frac{d}{d\lambda}\bar{F}_{PT}(q,\lambda) = \Big[U(\Lambda^2) + \frac{\omega}{\pi}E_1(\lambda\Lambda^2)\Big]\mathrm{e}^{-\lambda(q-\Lambda^2)}\,, \tag{2.37}$$

and

$$\frac{d^2}{d\lambda^2}\bar{F}_{PT}(q,\lambda) = -\frac{\omega}{\pi}\Big\{(q-\Lambda^2)\Big[E_1(\lambda\Lambda^2)+\frac{\pi}{\omega}U(\Lambda^2)\Big]+\frac{e^{-\lambda\Lambda^2}}{\lambda}\Big\}e^{-\lambda(q-\Lambda^2)}, \qquad (2.38)$$

allows us to deduce and plot the graphs of the possible cases governing the variation of $\bar{F}_{PT}(q,\lambda)$ against λ. These can be classified in the region $q > \Lambda^2$ according to the signs of the constants ω and $U(\Lambda^2)$ in the following way:

1. if $\omega > 0$ and $U(\Lambda^2) > 0$ then:

$$\frac{d}{d\lambda}\bar{F}_{PT}(q,\lambda) > 0 \qquad \text{and} \qquad \frac{d^2}{d\lambda^2}\bar{F}_{PT}(q,\lambda) < 0\,, \qquad \text{for } \lambda > 0\,,$$

which, in turn, imply that with increasing λ the curve of $\bar{F}_{PT}(q,\lambda)$ increases towards $F_{PT}(q)$ with a downward concavity as depicted in Fig.(2.4.1.a) and Fig.(2.4.1.b);

2. if $\omega > 0$ and $U(\Lambda^2) < 0$ then there is a local maximum at $\lambda = \lambda_{max}$, which can be deduced from:

$$\begin{aligned}\frac{d}{d\lambda}\bar{F}_{PT}(q,\lambda)\Big|_{\lambda=\lambda_{max}} &= 0 \implies E_1(\lambda_{max}\Lambda^2) = \frac{\pi}{\omega}|U(\Lambda^2)| \qquad \text{and}\\ \frac{d^2}{d\lambda^2}\bar{F}_{PT}(q,\lambda)\Big|_{\lambda=\lambda_{max}} &< 0\,;\end{aligned}$$

Here, the way in which $\bar{F}_{PT}(q,\lambda)$ approaches $F_{PT}(q)$ is different because $\bar{F}_{PT}(q,\lambda)$ rises first to the maximum $\bar{F}_{PT}(q,\lambda_{max})$ to fall next towards $F_{PT}(q)$ as λ increases beyond λ_{max} as shown in Fig.(2.4.2.a) and Fig.(2.4.2.b);

3. if $\omega < 0$ and $U(\Lambda^2) < 0$ then

$$\frac{d}{d\lambda}\bar{F}_{PT}(q,\lambda) < 0 \qquad \text{and} \qquad \frac{d^2}{d\lambda^2}\bar{F}_{PT}(q,\lambda) > 0\,, \qquad \text{for } \lambda > 0\,,$$

which indicates clearly that with increasing λ the curve of $\bar{F}_{PT}(q,\lambda)$ decreases towards $F_{PT}(q)$ with an upward concavity as depicted in Fig.(2.5.3.a) and Fig.(2.5.3.b);

4. if $\omega < 0$ and $U(\Lambda^2) > 0$ then there is a local minimum at $\lambda = \lambda_{min}$, which can be

deduced from:

$$\left.\frac{d}{d\lambda}\bar{F}_{PT}(q,\lambda)\right|_{\lambda=\lambda_{min}} = 0 \implies E_1(\lambda_{min}\Lambda^2) = \frac{\pi}{|\omega|}U(\Lambda^2) \qquad \text{and}$$
$$\left.\frac{d^2}{d\lambda^2}\bar{F}_{PT}(q,\lambda)\right|_{\lambda=\lambda_{min}} > 0;$$

Here, $\bar{F}_{PT}(q,\lambda)$ decreases in the direction of the minimum $\bar{F}_{PT}(q,\lambda_{min})$ as λ approaches λ_{min} from the left and begins to rise towards $F_{PT}(q)$ immediately after λ passes λ_{min} as shown in Fig.(2.5.4.a) and Fig.(2.5.4.b).

For each of these four cases, there corresponds two possibilities either

$$\text{(a)} \qquad F(q) < F_{PT}(q) \qquad \text{or},$$
$$\text{(b)} \qquad F(q) > F_{PT}(q).$$

Accordingly, we shall denote the case associated with either possibility by case(i.a) or case(i.b) with $i = 1, 2, 3$ or 4. These cases are illustrated in Fig.(2.4) and Fig.(2.5). In these figures, we include for each case an illustrative hypothetical graph for $\bar{F}(q,\lambda)$ based on our knowledge of the small and large behaviour of $\bar{F}(q,\lambda)$, i.e. $\bar{F}(q,\lambda) \cong \bar{F}_{PT}(q,\lambda)$ for sufficiently small λ and $\bar{F}(q,\lambda) \cong F(q)$ for large enough λ. In applying our method we will need to know *a priori* whether $F_{PT}(q)$ is less than or greater than $F(q)$, either by input from an experiment or by a knowledge of the signs of higher order corrections to the perturbation theory in a regime where this can be trusted.

Our choice of λ_0 for the different cases, at a fixed value $q > \Lambda^2$, is as follows:

1. in case(1.a), the ideal value of λ_0 is the one at which $\bar{F}_{PT}(q,\lambda)$ intersects with $F(q)$ as shown in Fig.(2.4.1.a); such a point is not precisely known although it may be estimated from a knowledge of higher order corrections to F_{PT} if these are available. We expect it to occur near the point of greatest curvature of $\bar{F}_{PT}(q,\lambda)$ as illustrated by the shaded region in Fig.(2.4.1.a). So for this case we might alternatively take λ_0 to be the value of λ where the curvature is greatest.

2. in case(1.b), the monotonicity of $\bar{F}_{PT}(q,\lambda)$ means that sampling this curve at any finite value of λ will fail to improve the perturbative estimate. However the use of a large, but finite value will depart little from the perturbative estimate (as the

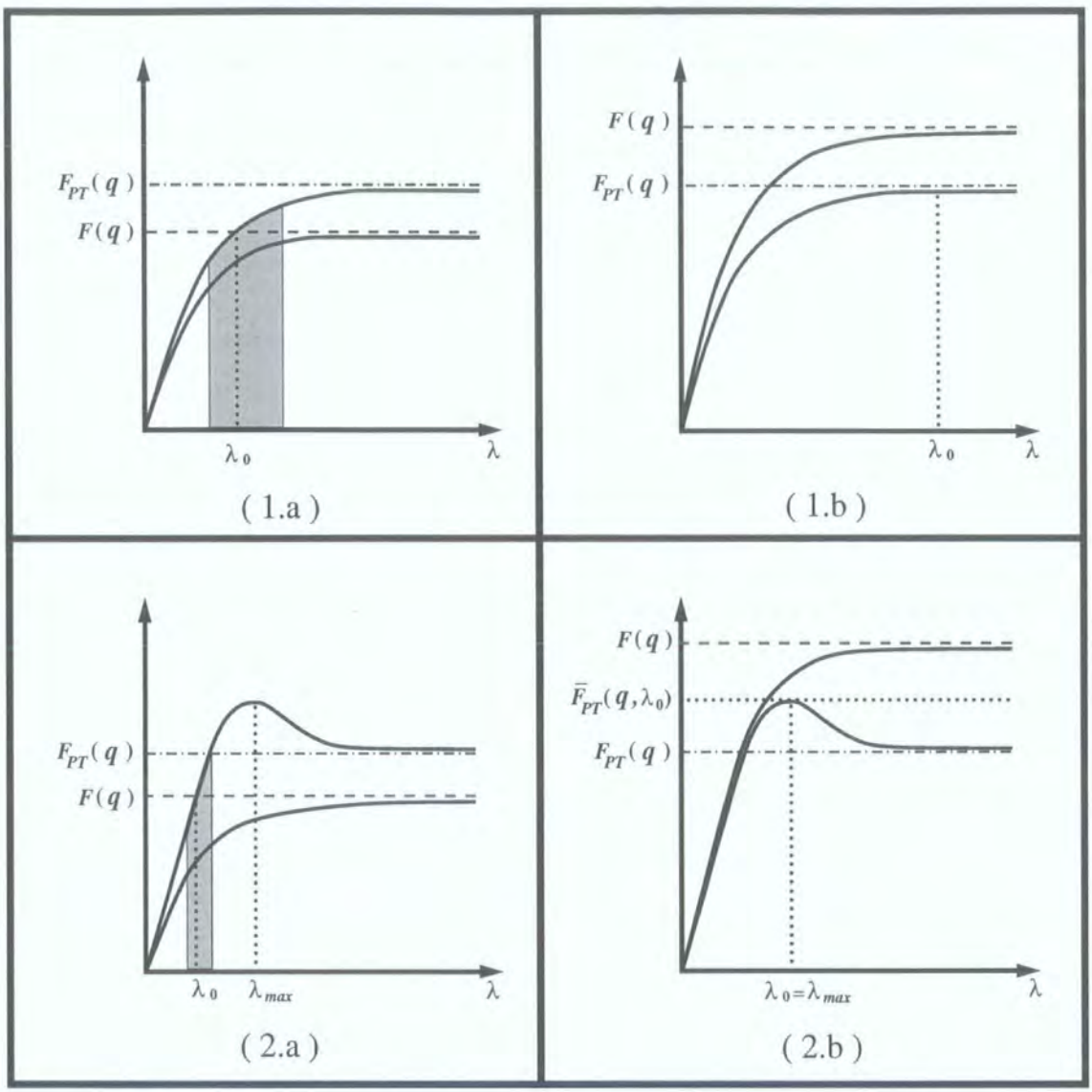


Figure 2.4: The variation of $\bar{F}_{PT}(q,\lambda)$ and the expected $\bar{F}(q,\lambda)$ versus λ at a fixed value $q > \Lambda^2$. In (1.a) and (2.a) the upper and the lower curves describe $\bar{F}_{PT}(q,\lambda)$ and $\bar{F}(q,\lambda)$ respectively. In (1.b) and (2.b) the upper and the lower curves describe $\bar{F}(q,\lambda)$ and $\bar{F}_{PT}(q,\lambda)$ respectively.

asymptotic behaviour is approached rapidly) and will have the merit of reinstating causality. So our best choice for λ_0 is the smallest $\lambda-$value at which $\bar{F}_{PT}(q,\lambda)$ is acceptably close to $F_{PT}(q)$.

3. in case(2.a), the ideal value of λ_0 is the one at which $\bar{F}_{PT}(q,\lambda)$ intersects with $F(q)$ as shown in Fig.(2.4.2.a); such a point is expected to lie within a narrow domain, on the left of λ_{max}, corresponding to a small arc segment just below $F_{PT}(q)$ as

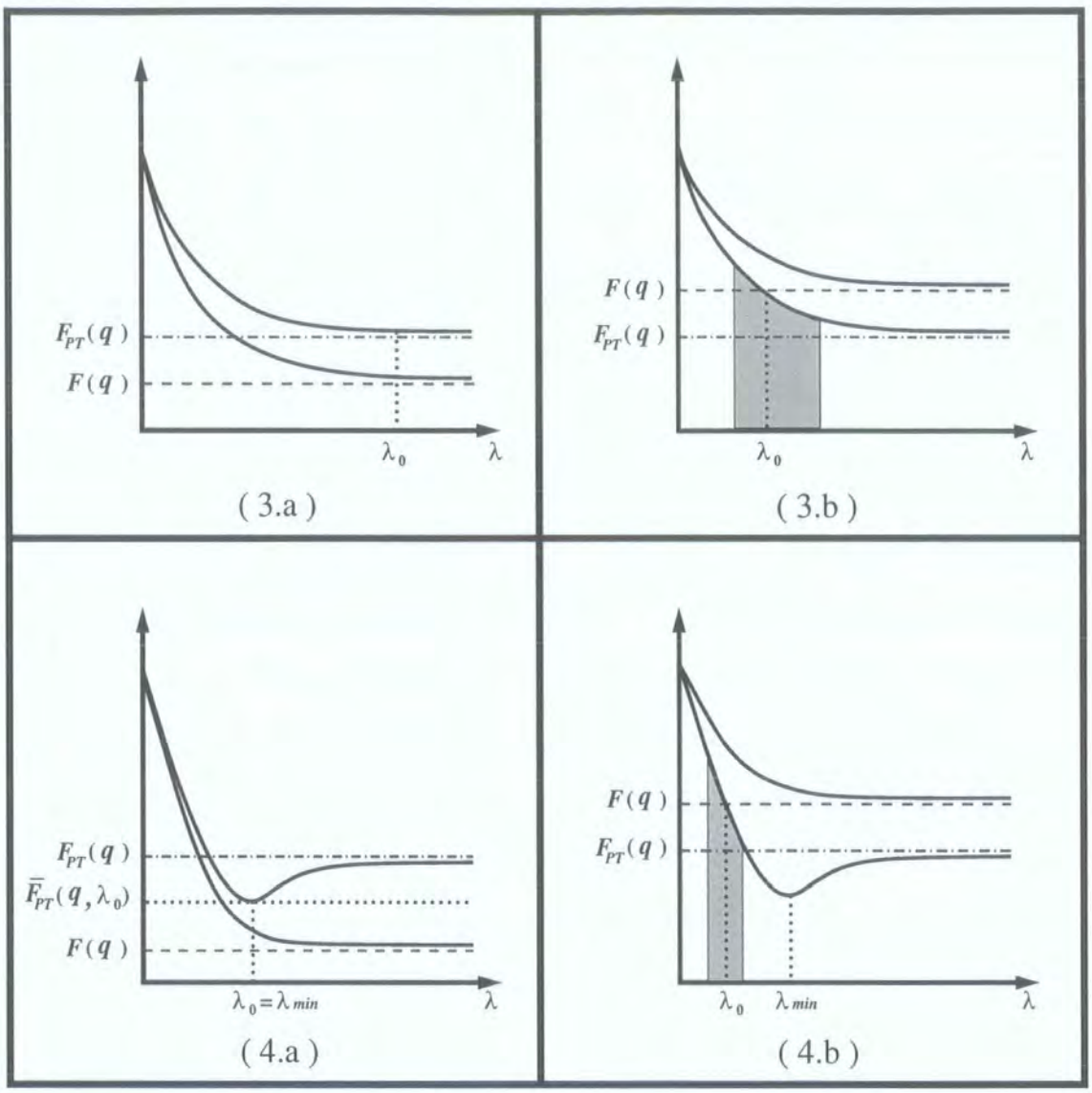


Figure 2.5: The variation of $\bar{F}_{PT}(q,\lambda)$ and the expected $\bar{F}(q,\lambda)$ versus λ at a fixed value $q > \Lambda^2$. In (3.a) and (4.a) the upper and the lower curves describe $\bar{F}_{PT}(q,\lambda)$ and $\bar{F}(q,\lambda)$ respectively. In (3.b) and (4.b) the upper and the lower curves describe $\bar{F}(q,\lambda)$ and $\bar{F}_{PT}(q,\lambda)$ respectively.

illustrated by the shaded region in Fig.(2.4.2.a); such a point might be estimated from a knowledge of higher order perturbative corrections; however without further information it is not possible to see how to identify this region from a knowledge of the perturbative function $\bar{F}_{PT}(q,\lambda)$ alone.

4. in case(2.b), the best choice for λ_0 is λ_{max}, as illustrated in Fig.(2.4.2.b), and this leads to an improvement over the perturbative estimate.

The cases depicted in Fig.(2.5) differ essentially by just a sign change, so a similar discussion of the appropriate choice of λ_0 can be made.

To summarise, from a *prior* knowledge of whether the perturbative estimate overshoots or undershoots the true value of the observable $F(q)$, and by plotting the shape of $\bar{F}_{PT}(q,\lambda)$ against λ we can ascertain which of the various possible cases occurs in a given situation. For cases (1.a), (2.a), (3.b) and (4.b), there exists a unique point $\lambda = \lambda_0$ at which $\bar{F}_{PT}(q,\lambda_0)$ matches the observable $F(q)$. However, for cases (2.b) and (4.a) the situation is different but still there is a point λ_0 at which $\bar{F}_{PT}(q,\lambda_0)$ can give a bitter result than that of perturbation theory. In these cases, we can estimate λ_0 from the properties of $\bar{F}_{PT}(q,\lambda)$, or with the aid of higher order perturbative corrections, in a way that will improve on the perturbative predictions. On the other hand, in the remaining two cases (1.b) and (3.a) such an improvement does not occur.

Having determined λ_0 as a function of q in a domain where perturbation theory is reasonably trustworthy, we use its average λ_e in $\bar{F}_{PT}(q,\lambda_e)$ to extrapolate to smaller values of q. This results in an estimate free of the unphysical divergences of the original perturbative approximation, and this is the central goal of our approach. This will be true even for the cases (1.b) and (3.a). In some cases, the effective average value λ_e is either equal to or not significantly different from $\lambda_0(q)$. This is always true if $\lambda_0(q)$ is either a constant or a slowly varying function over a large domain of q. For instance, in our illustrative example λ_e assumes the value λ_{max} in case(2.b) and λ_{min} in case(4.a); in other words it coincides with $\lambda_0(q)$ for all $q > \Lambda^2$. Also, it follows from the inequality:

$$|\Upsilon_{IR}(q,\lambda_e)| \leq \frac{|U(\Lambda^2)|}{q-\Lambda^2}\ \mathrm{e}^{-\lambda_e(q-\Lambda^2)} + \frac{|\omega|}{\pi\Lambda^2}\ \frac{\mathrm{e}^{-\lambda_e q}}{\lambda_e\, q} \qquad \text{for } q \neq \Lambda^2\,, \tag{2.39}$$

that the contribution of $\Upsilon_{IR}(q,\lambda_e)$ becomes negligible for $q \gg \Lambda^2$. Hence, employing λ_e in the remote UV region does not spoil the standard perturbative results.

One final point to remark is that the method also applies in the reverse direction to the previous setting. For example, in the case when the infrared behaviour $F_{IR}(q)$ is well known then a similar representation to (2.1), but with q replaced by a variable with the dimensions of length squared $r = 1/q$, can be used in almost the same way as before except

this time to deduce the corresponding analytic UV expression:

$$\bar{F}_{UV}(q,\lambda) = \frac{1}{2\pi i}\int_{C_{IR}} \frac{e^{\lambda(\bar{r}-r)}}{\bar{r}-r}\, F_{IR}(1/\bar{r})\, d\bar{r}\,. \tag{2.40}$$

From this viewpoint, our method plays the role of a bridge between regions of small and large momenta, allowing us from a *prior* knowledge of either the UV or IR behaviour to extract information about the IR or UV properties respectively.

2.2 Analysis of the one-loop QCD running coupling

In this section, we demonstrate the implementation of our method in constructing a simple model for describing the regular IR behaviour of the QCD effective coupling constant. For ease of calculation, we assume that the zeros of the exact function $\alpha(Q^2)$ of the running coupling are expected to occur only on the negative real axis $\mathrm{Re}\{Q^2\} < 0$ and/or infinity. This, together with the causality principle, allows us to express the reciprocal of $\alpha(Q^2)$ in terms of the contour integral:

$$\frac{1}{\alpha(Q^2)} = \frac{1}{2\pi i}\lim_{\lambda\to\infty}\int_{C_{UV}} \frac{e^{\lambda(k-Q^2)}}{k-Q^2}\,\frac{1}{\alpha(k)}\, dk\,, \tag{2.41}$$

introduced in the previous section. When applying this representation to an n-loop perturbative expression $\alpha^{(n)}_{\mathrm{PT}}(Q^2)$, we take $\lambda = \lambda_e$ instead of ∞. In this way, we obtain a combination of perturbative and non-perturbative contributions, which has the merit of:

1. reinstating the causal analyticity structure in the right half plane $\mathrm{Re}\{Q^2\} \geq 0$,
2. preserving the standard UV behaviour and,
3. improving the perturbative estimate in both the IR and low UV regions.

In the following, we shall prove this claim within the one-loop approximation. For convenience, we express the reciprocal of $\alpha^{(1)}_{\mathrm{PT}}(Q^2)$ in terms of a dimensionless variable $q = Q^2/\Lambda^2$ as:

$$\frac{1}{\alpha^{(1)}(q)} = \frac{\beta_0}{4\pi}\ln(q)\,, \tag{2.42}$$

where [1] $\alpha^{(1)}(Q^2/\Lambda^2) = \alpha^{(1)}_{\rm PT}(Q^2)$. In the spirit of (2.41), an analytically improved expression corresponding to the one-loop coupling constant can be defined as:

$$\bar{\alpha}^{(1)}(q,\lambda_e) = \left.\frac{1}{\bar{\chi}^{(1)}(q,\lambda)}\right|_{\lambda=\lambda_e}, \tag{2.43}$$

with

$$\bar{\chi}^{(1)}(q,\lambda) = \frac{1}{2\pi i}\int_{C_{UV}} \frac{e^{\lambda(k-q)}}{k-q}\,\frac{1}{\alpha^{(1)}(k)}\,dk\,. \tag{2.44}$$

Note that since $[\alpha^{(1)}(k)]^{-1}$ depends on $1/\ln q$ it has a cut along the negative real axis $\mathrm{Re}\{k\} \leq 0$. We shall now proceed to evaluate the above integral for the case $q \neq 0$. Following the same argument of the preceding section from (2.1) to (2.4), we can show that:

$$\bar{\chi}^{(1)}(q,\lambda) = \frac{\beta_0}{4\pi}\ln(q) + \frac{\beta_0}{4\pi} I_{C_k}(q,\lambda)\,, \tag{2.45}$$

where

$$I_{C_k}(q,\lambda) = \mathrm{J}_\epsilon(q,\lambda) + \int_\epsilon^{R_{\rm UV}} \frac{e^{-\lambda(k+q)}}{k+q}\,dk\,, \tag{2.46}$$

with

$$\mathrm{J}_\epsilon(q,\lambda) = \frac{\epsilon\, e^{-\lambda q}}{2\pi}\int_{-\pi}^{\pi} e^{\lambda\epsilon\cos(\theta)}\,\mathrm{Re}\left(\frac{e^{i\lambda\epsilon\sin(\theta)}\,\ln(\epsilon\, e^{i\theta})}{\epsilon - q\, e^{-i\theta}}\right) d\theta\,. \tag{2.47}$$

A simple way to check that the contribution of $\mathrm{J}_\epsilon(q,\lambda)$ vanishes as ϵ approaches zero is to consider the upper bound:

$$|\mathrm{J}_\epsilon(q,\lambda)| \leq \frac{e^{-\lambda(q-\epsilon)}}{(q-\epsilon)}\,\epsilon\,\left(\ln^2(\epsilon)+\pi^2\right)^{1/2}, \tag{2.48}$$

from which it follows that:

$$\lim_{\epsilon\to 0} \mathrm{J}_\epsilon(q,\lambda) = 0\,. \tag{2.49}$$

Consequently, in the limit as $\epsilon \to 0$ we can write in a simple form:

$$I_{C_k}(q,\lambda) = \int_0^{R_{\rm UV}} \frac{e^{-\lambda(k+q)}}{k+q}\,dk \;= E_1(\lambda q) - E_1(\lambda(q+R_{\rm UV}))\,. \tag{2.50}$$

[1] In this thesis, we use the notation $\alpha^{(n)}(q = Q^2/\Lambda^2) = \alpha^{(n)}_{\rm PT}(Q^2)$ for the corresponding n-loop approximation.

By inserting this into (2.45) and letting $R_{\rm UV} \to \infty$, we obtain:

$$\bar{\chi}^{(1)}(q,\lambda) = \frac{\beta_0}{4\pi}\Big[\,\ln(q) + E_1(\lambda\, q)\Big]\,. \tag{2.51}$$

Having found the exact structure of $\bar{\chi}^{(1)}(q,\lambda)$ for $q \neq 0$, let us now reconsider the contour integral (2.44) once more to explore the continuity of $\bar{\chi}^{(1)}(q,\lambda)$ at the origin of q. Starting from the expression:

$$\bar{\chi}^{(1)}(0,\lambda) = \frac{\beta_0}{4\pi}\frac{1}{2\pi i}\int_{C_{UV}} \frac{\mathrm{e}^{\lambda k}}{k}\,\ln(k)\,dk\,, \tag{2.52}$$

we arrive, after some work, at

$$\begin{aligned}\bar{\chi}^{(1)}(0,\lambda) = &\frac{\beta_0}{4\pi}\lim_{\epsilon\to 0}\Bigg[\int_\epsilon^{R_{\rm UV}} \frac{\mathrm{e}^{-\lambda k}}{k}\,dk + \frac{\ln(\epsilon)}{\pi}\int_0^\pi \mathrm{e}^{\lambda\epsilon\cos(\theta)}\,\cos(\lambda\epsilon\sin(\theta))\,d\theta \\ &- \frac{1}{\pi}\int_0^\pi \mathrm{e}^{\lambda\epsilon\cos(\theta)}\,\sin(\lambda\epsilon\sin(\theta))\,\theta\,d\theta\Bigg]\,.\end{aligned} \tag{2.53}$$

Making use of

$$\int_\epsilon^{R_{\rm UV}} \frac{\mathrm{e}^{-\lambda k}}{k}\,dk = E_1(\lambda\epsilon) - E_1(\lambda R_{\rm UV})\,, \tag{2.54}$$

and inserting the following series representations [51]:

$$\begin{aligned}\mathrm{e}^{\lambda\epsilon\cos(\theta)}\,\cos(\lambda\epsilon\sin(\theta)) &= \sum_{n=0}^{\infty}\frac{(\lambda\epsilon)^n}{n!}\,\cos(n\theta) \qquad \text{for } \lambda\epsilon < 1\,,\\ \mathrm{e}^{\lambda\epsilon\cos(\theta)}\,\sin(\lambda\epsilon\sin(\theta)) &= \sum_{n=1}^{\infty}\frac{(\lambda\epsilon)^n}{n!}\,\sin(n\theta) \qquad \text{for } \lambda\epsilon < 1\,,\end{aligned}$$

into the two angular integrals in (2.53), we immediately obtain:

$$\bar{\chi}^{(1)}(0,\lambda) = \frac{\beta_0}{4\pi}\lim_{\epsilon\to 0}\Bigg[E_1(\lambda\epsilon) - E_1(\lambda R_{\rm UV}) + \ln(\epsilon) + \sum_{n=1}^{\infty}\frac{(-1)^n}{n!\,n}\,(\lambda\epsilon)^n\Bigg]\,. \tag{2.55}$$

If we now make use of (2.21) and let $R_{\rm UV} \to \infty$, we arrive at:

$$\bar{\chi}^{(1)}(0,\lambda) = \frac{\beta_0}{4\pi}\,\ln(\mathrm{e}^{-\gamma_{\rm E}}/\lambda)\,. \tag{2.56}$$

This ensures the continuity condition at the origin:

$$\lim_{q\to 0} \bar{\chi}^{(1)}(q,\lambda) = \bar{\chi}^{(1)}(0,\lambda)\,. \tag{2.57}$$

Let us now find the range of λ for which:

$$\bar{\alpha}^{(1)}(q,\lambda) = \frac{1}{\bar{\chi}^{(1)}(q,\lambda)} = \frac{4\pi}{\beta_0}\,\frac{1}{[\,\ln(q) + E_1(\lambda\, q)\,]}\,, \tag{2.58}$$

is continuous on the whole interval $q \geq 0$. This requires an investigation of the zeros of $\bar{\chi}^{(1)}(q,\lambda)$ in $D_{\bar{\chi}}$, where $D_{\bar{\chi}} = \{(q,\lambda) : q \geq 0,\ \lambda > 0\}$. From expression (2.51), we know that since $E_1(\lambda\, q) > 0$ in $D_{\bar{\chi}}$ and $\ln q$ is negative only when $q \in (0,1)$, the zeros of $\bar{\chi}^{(1)}(q,\lambda)$ are expected to occur somewhere in the subinterval $\{(q,\lambda) : 0 \leq q < 1,\ \lambda > 0\} \subset D_{\bar{\chi}}$. This domain can be reduced further by first considering the complementary exponential integral:

$$Ein(x) = \int_0^1 \frac{[1 - \mathrm{e}^{-xt}]}{t}\, dt = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n}\,\frac{x^n}{n!}\,, \qquad x \geq 0\,, \tag{2.59}$$

to rewrite (2.51) as:

$$\bar{\chi}^{(1)}(q,\lambda) = \frac{\beta_0}{4\pi}\,[\,\ln(\mathrm{e}^{-\gamma_{\mathrm{E}}}/\lambda) + Ein(\lambda\, q)\,]\,. \tag{2.60}$$

Then by observing the fact that $Ein(\lambda\, q) \geq 0$ for all $\lambda\, q \geq 0$ and that $\ln(\mathrm{e}^{-\gamma_{\mathrm{E}}}/\lambda) < 0$ only if $\lambda > \mathrm{e}^{-\gamma_{\mathrm{E}}}$, we deduce that the zeros of $\bar{\chi}^{(1)}(q,\lambda)$ can exist only in the following interval $\{(q,\lambda) : 0 \leq q < 1,\ \lambda \geq \mathrm{e}^{-\gamma_{\mathrm{E}}}\}$. Hence, $\bar{\alpha}^{(1)}(q,\lambda)$ is continuous for all $q \geq 0$ if and only if $\lambda \in (0, \mathrm{e}^{-\gamma_{\mathrm{E}}})$. Another way to obtain this result is by considering the fact that $\bar{\alpha}^{(1)}(0,\lambda) \geq \bar{\alpha}^{(1)}(q,\lambda)$ for all values of λ that keep $\bar{\alpha}^{(1)}(q,\lambda)$ finite and positive throughout the range $q \geq 0$. Then, from the positivity of:

$$\bar{\alpha}^{(1)}(0,\lambda) = \frac{4\pi}{\beta_0}\,\frac{1}{\ln(\mathrm{e}^{-\gamma_{\mathrm{E}}}/\lambda)}\,, \tag{2.61}$$

it follows that the allowed values of λ are those confined to the interval:

$$D_{eff} = \{\lambda\ :\ 0 < \lambda < \mathrm{e}^{-\gamma_{\mathrm{E}}} \approx 0.561\}\,. \tag{2.62}$$

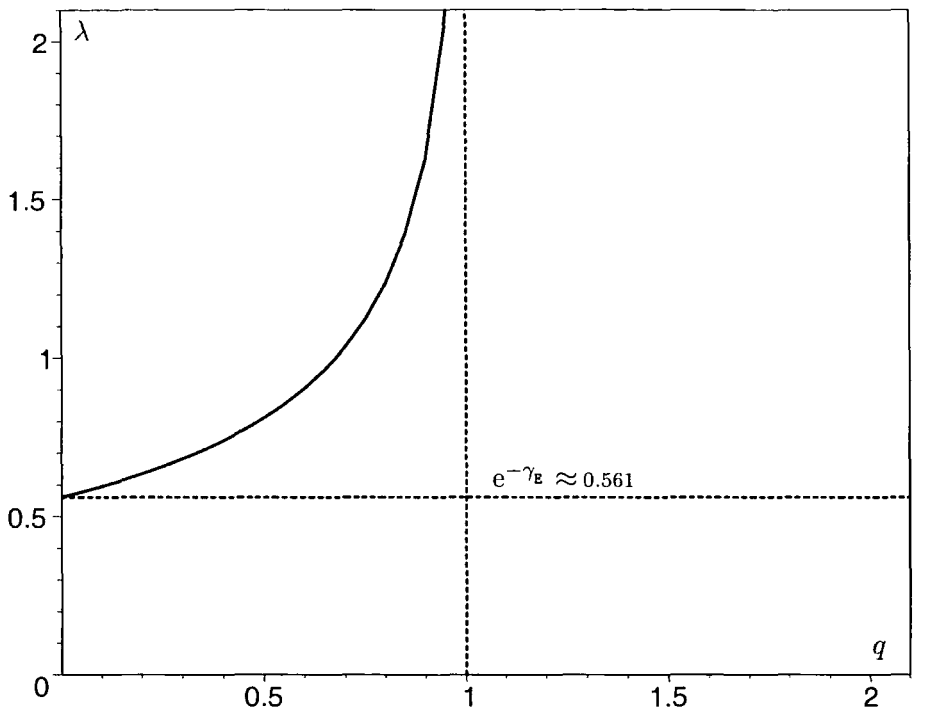


Figure 2.6: The zeros of $\bar{\chi}^{(1)}(q,\lambda)$: the curve shown in the strip $\{(q,\lambda) : 0 \leq q < 1,\ \lambda \geq e^{-\gamma_E}\}$ represents the roots of $\bar{\chi}^{(1)}(q,\lambda)$ in $D_{\bar{\chi}}$. This curve never touches the vertical $q = 1$ as $\bar{\chi}^{(1)}(q,\lambda)$ does not have a zero on this line.

Using Maple VI for solving $\bar{\chi}^{(1)}(q,\lambda) = 0$ numerically, we illustrate in Fig.(2.6) the zeros of $\bar{\chi}^{(1)}(q,\lambda)$, i.e the singularities of $\bar{\alpha}^{(1)}(q,\lambda)$, by a curve confined to the strip $\{(q,\lambda) : 0 \leq q < 1,\ \lambda \geq e^{-\gamma_E}\}$, showing that D_{eff} is the only region of λ for which $\bar{\alpha}^{(1)}(q,\lambda)$ is continuous for all $q \geq 0$.

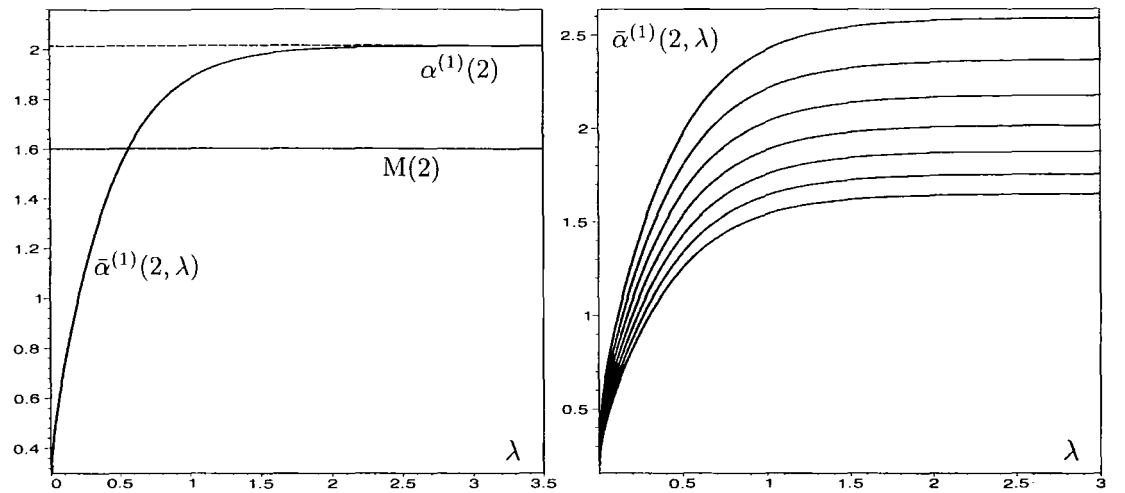
2.3 The Estimation of λ_e

In this section, we try to find an effective value $\lambda_e \in D_{eff}$ such that $\bar{\alpha}^{(1)}(q,\lambda_e)$ provides a better estimate than that of the standard perturbative results, especially in the vicinity of the Landau-pole and the IR region.

From the constraint (2.62), it follows that:

$$0 < \bar{\alpha}^{(1)}(q,\lambda_e) < \mathrm{M(q)} \qquad \text{for all } q \geq 0\,, \tag{2.63}$$

where the upper bound $\mathrm{M(q)} = \bar{\alpha}^{(1)}(q, \mathrm{e}^{-\gamma_E})$. This implies that $\bar{\alpha}^{(1)}(q,\lambda_e) < \alpha^{(1)}(q) = \bar{\alpha}^{(1)}(q,\lambda \gg 1)$ for all $q > 1$. However, since $E_1(\lambda_e\, q)$ in (2.58) is negligibly small for $q \gg \lambda_e$,



(a) (b)

Figure 2.7: The variation of $\bar{\alpha}^{(1)}(2,\lambda)$ versus λ, (a) for $n_f = 3$ and (b) for $0 \leq n_f \leq 6$. Here, $\bar{\alpha}^{(1)}(2,\lambda)$ tends to $\alpha^{(1)}(2)$ as λ increases. In (b), $\bar{\alpha}^{(1)}(2,\lambda)$ increases with n_f for any fixed value of λ.

we may consider $\bar{\alpha}^{(1)}(q,\lambda_e) = \alpha^{(1)}(q)$ at sufficiently large values of q. For a given n_f and $q > 1$, we find that the way in which $\bar{\alpha}^{(1)}(q,\lambda)$ changes with λ, as shown in Fig.(2.7), is a typical example of case(1) illustrated in Fig.(2.4). Hence, before setting up a criterion for determining λ_e, we need to find out whether the perturbative estimate $\alpha^{(1)}(q)$, in the low UV region, overshoots or undershoots the true value $\alpha(q)$. This can be deduced by comparing $\alpha^{(1)}(q)$ to the standard higher-loop corrections [29]:

$$\alpha^{(2)}(q) = \frac{4\pi}{\beta_0 L}\left[1 - \frac{\beta_1}{\beta_0^2}\frac{\ln L}{L}\right], \tag{2.64}$$

and

$$\alpha^{(3)}(q) = \frac{4\pi}{\beta_0 L}\left[1 - \frac{\beta_1}{\beta_0^2}\frac{\ln L}{L} + \frac{\beta_1^2 \ln^2 L - \beta_1^2 \ln L + \beta_2\beta_0 - \beta_1^2}{\beta_0^4 L^2}\right], \tag{2.65}$$

where $L = \ln q$ with $q = Q^2/\Lambda^2$, and [30]:

$$\beta_1 = 102 - \frac{38}{3} n_f, \tag{2.66}$$

$$\beta_2 = \frac{2857}{2} - \frac{5033}{18} n_f + \frac{325}{54} n_f^2. \tag{2.67}$$

Fig.(2.8) illustrates the comparison in terms of the physical scale Q [GeV]. In this figure, we consider $n_f = 3$ and take $\Lambda = 0.593$ GeV, 0.495 GeV and 0.383 GeV for $\alpha^{(1)}_{\rm PT}(Q^2)$, $\alpha^{(2)}_{\rm PT}(Q^2)$ and $\alpha^{(3)}_{\rm PT}(Q^2)$ respectively. The Λ values are determined in the $\overline{\rm MS}$ scheme from

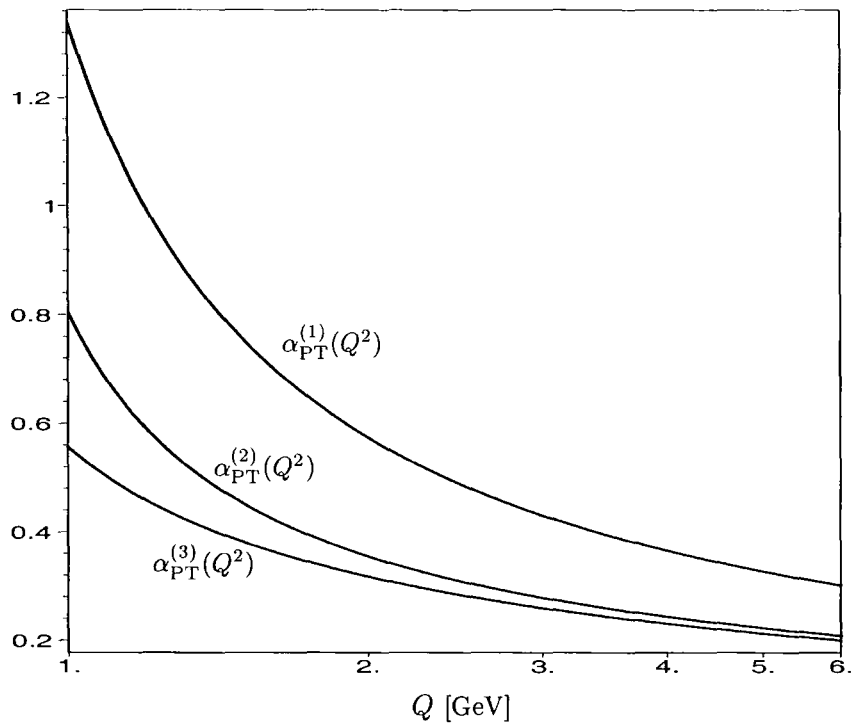


Figure 2.8: The comparison between the 1-, 2- and 3-loop running coupling for $n_f = 3$, showing that $\alpha_{\rm PT}^{(1)}(Q^2) > \alpha_{\rm PT}^{(2)}(Q^2) > \alpha_{\rm PT}^{(3)}(Q^2)$.

the experimentally measured $\tau-$lepton decay rate [31] given by:

$$R_\tau = 2.9087\,(0.998 + \delta_p^{(n)}) = 3.492\,, \tag{2.68}$$

where

$$\delta_p^{(n)} = \sum_{k=1}^{n} a_k \left(\frac{\alpha_{\rm PT}^{(n)}(M_\tau^2)}{\pi}\right)^k . \tag{2.69}$$

Here $n \leq 3$ denotes the n^{th} loop order approximation, $a_1 = 1$, $a_2 = 5.20232$, $a_3 = 26.3659$ and $M_\tau = 1.777$ GeV. In Fig.(2.8), we used $n_f = 3$ as the average number of active quarks, ignoring complications due to quark thresholds. This is reasonable in the low energy interval $Q < 3$ GeV. For a more precise description of the evolution of $\alpha_{\rm PT}^{(n)}(Q^2)$ in a larger momentum interval, one should take into account the effects of quark thresholds. However, this does not change the overall picture illustrated in Fig.(2.8). Having now observed that $\alpha_{\rm PT}^{(1)}(Q^2) > \alpha_{\rm PT}^{(2)}(Q^2) > \alpha_{\rm PT}^{(3)}(Q^2)$, we would expect $\alpha^{(1)}(q)$ to overshoot the true value of the coupling constant, at least for intermediate and sufficiently small values of q. This indicates that our problem is of the type classified earlier as case(1.a) and

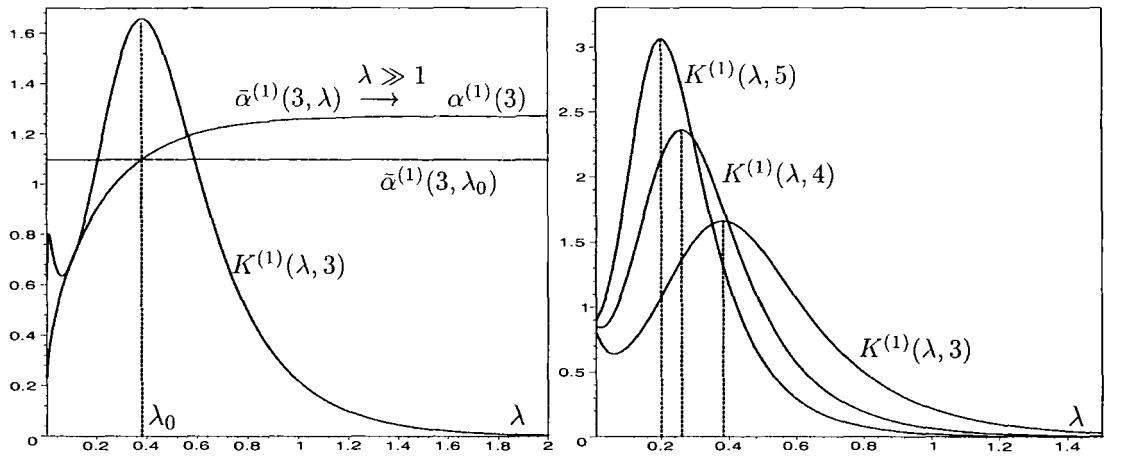


Figure 2.9: The variation of $K^{(1)}(\lambda;q)$ versus λ for $n_f = 3$, (a) at $q = 3$ and (b) at $q = 3,4,5$. For a fixed $q > 1$, $\lambda_0(q)$ denotes the value of λ at which $K^{(1)}(\lambda;q)$ is a local maximum. In (b), $\lambda_0(5) < \lambda_0(4) < \lambda_0(3)$.

depicted in Fig.(2.4.1.a). Hence, we may ascertain that for every point $q > 1$ there exists a proper value $\lambda_0(q)$ such that $\bar{\alpha}^{(1)}(q,\lambda_0(q)) = \alpha(q)$, just as explained in case(1.a). One way to estimate $\lambda_0(q)$ is to first consider the curvature function of $\bar{\alpha}^{(1)}(q,\lambda)$:

$$K^{(1)}(\lambda,q) = \frac{|\bar{\alpha}^{(1)}_{\lambda\lambda}(q,\lambda)|}{\left[1 + (\bar{\alpha}^{(1)}_{\lambda}(q,\lambda))^2\right]^{3/2}}, \tag{2.70}$$

for a fixed $q > 1$, where

$$\bar{\alpha}^{(1)}_{\lambda}(q,\lambda) = \frac{\partial}{\partial\lambda}\bar{\alpha}^{(1)}(q,\lambda) = \frac{\beta_0}{4\pi}\left[\bar{\alpha}^{(1)}(q,\lambda)\right]^2 \frac{e^{-\lambda q}}{\lambda}, \tag{2.71}$$

$$\bar{\alpha}^{(1)}_{\lambda\lambda}(q,\lambda) = \frac{\partial^2}{\partial\lambda^2}\bar{\alpha}^{(1)}(q,\lambda) = \bar{\alpha}^{(1)}_{\lambda}(q,\lambda)\left[\frac{\beta_0}{2\pi}\,\bar{\alpha}^{(1)}(q,\lambda)\,\frac{e^{-\lambda q}}{\lambda} - \frac{1}{\lambda} - q\right]. \tag{2.72}$$

Then take $\lambda_0(q)$ to be the value of λ at which $K^{(1)}(\lambda_0,q)$ is a local maximum. For sufficiently small values of $q > 1$, $K^{(1)}(\lambda,q)$ has two local maxima, say at λ_1 and λ_2. In this case, we consider λ_0 to be the largest of these (say $\lambda_0 = \lambda_2 > \lambda_1$) so that $\bar{\alpha}^{(1)}(q,\lambda_0)$ remains as close as possible to the perturbative results $\alpha^{(1)}(q)$, which are still reasonable for such values of q. In Fig.(2.9) we plot the curvature function $K^{(1)}(\lambda,q)$ versus λ for some fixed values of q, illustrating in part (a) of the figure the difference between $\bar{\alpha}^{(1)}(q,\lambda_0)$ and $\alpha^{(1)}(q)$ for $q = 3$. In part (b) of Fig.(2.9), we observe that the value of λ_0 decreases with increasing q. In general, if we plot λ_0 against q for any quark flavour n_f we find that

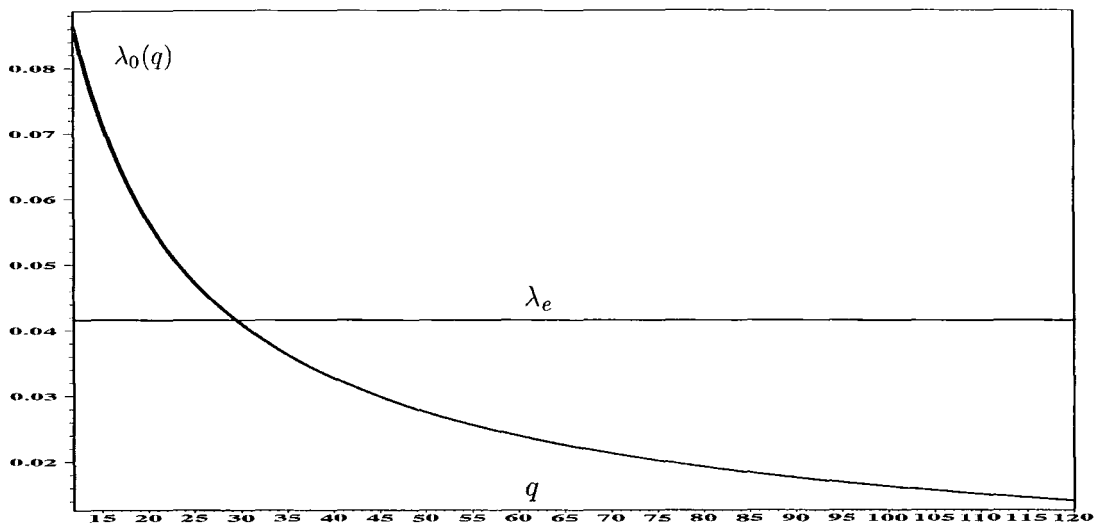


Figure 2.10: The variation of $\lambda_0(q)$ versus q, for $n_f = 3$.

$\lambda_0(q)$ is a monotonically decreasing function as shown in Fig.(2.10) for $n_f = 3$. Hence, we may express D_{eff} in terms of $\lambda_0(q)$ as follows:

$$D_{eff} = \{\lambda : \lambda_0(\infty) < \lambda < \lambda_0(q_0)\},$$

with q_0 defined by $\lambda_0(q_0) = e^{-\gamma_E}$. The values of q_0 for different n_f are all given in table(2.1). For sufficiently large values of q, our choice of λ_0 does not lead to a significant

n_f	0	1	2	3	4	5	6
q_0	2.204	2.246	2.293	2.345	2.402	2.467	2.539

Table 2.1: Numerical values of $q_0(n_f)$

improvement on the perturbative estimate. In fact, since only the first two decimal places of the coupling constant are of physical interest, we may take $\bar{\alpha}^{(1)}(q, \lambda_0(q)) \cong \alpha^{(1)}(q)$ for all $q \geq 120$ and $0 \leq n_f \leq 6$. On this basis, we shall focus our attention on the effective domain:

$$S_{eff} = \{\, q : \; q_0 < q < 120 \,\}, \tag{2.73}$$

over which the difference between $\bar{\alpha}^{(1)}(q, \lambda_0(q))$ and $\alpha^{(1)}(q)$ is appreciable. Thus, we expect to find λ_e in a narrower interval, $\bar{D}_{eff} = \{\lambda : \lambda_0(120) < \lambda < \lambda_0(q_0)\} \subset D_{eff}$. Since, as illustrated in Fig.(2.10), $\lambda_0(q)$ is a very slowly varying function over a large part of the interval S_{eff}, i.e. for $q \in (11, 120)$, we take the average of $\lambda_0(q)$ over S_{eff} to be the

best estimated value for λ_e. Our numerical results for λ_e are listed in table(2.2) for the n_f values of practical interest. As seen from table(2.2), the values of λ_e do not change

n_f	0	1	2	3	4	5	6
λ_e	0.0379	0.0390	0.0402	0.0416	0.0429	0.0444	0.0461

Table 2.2: Numerical values of $\lambda_e(n_f)$

appreciably with n_f. Hence, we shall fix λ_e to a central value of 0.04 for all values of n_f.

Let us now denote $\bar{\alpha}^{(1)}(Q^2/\Lambda^2, \lambda_e)$ by $\bar{\alpha}^{(1)}(Q^2)$, where:

$$\bar{\alpha}^{(1)}(Q^2) = \frac{4\pi}{\beta_0} \frac{1}{[\,\ln(Q^2/\Lambda^2) + E_1(\lambda_e\, Q^2/\Lambda^2)\,]}\,. \tag{2.74}$$

In this expression, the exponential integral function $E_1(\lambda_e\, Q^2/\Lambda^2)$ plays an important role in removing the ghost pole at $Q = \Lambda$, preserving the correct UV behaviour (as it decays rapidly to zero for $Q \gg \Lambda$) and enforcing the running coupling to freeze in the low IR region. Therefore, it is essentially non-perturbative. At low energies, $\bar{\alpha}^{(1)}(Q^2)$ approximates well to the simple formula:

$$\bar{\alpha}^{(1)}(Q^2) = \frac{4\pi}{\beta_0\, \kappa_e} \frac{\varpi^2}{\varpi^2 + Q^2} \qquad \text{for} \quad 0 \leq Q^2 \leq \Lambda^2\,, \tag{2.75}$$

where $\kappa_e = \ln(e^{-\gamma_E}/\lambda_e)$ and $\varpi^2 = \kappa_e\, \Lambda^2/\lambda_e$. In particular, this yields a finite value at the origin, namely:

$$\bar{\alpha}^{(1)}(0) = \frac{4\pi}{\beta_0\, \kappa_e}\,, \tag{2.76}$$

which is totally independent of the characteristic mass scale Λ. Obviously, this is a key advantage of our approach as it agrees with the IR freezing phenomenological hypothesis [22, 24]. Now, let me remark from Ref. [24] that the freezing phenomenon is not incompatible with confinement as there is no evidence that confinement necessarily requires the coupling constant to become infinite in the IR region. For instance, Gribov's ideas on confinement [23–26] explicitly involve a freezing of the coupling constant at low momenta. This phenomenon is also present in perturbation theory but beyond the leading order and for certain numbers of quark flavours.

Chapter 3

Empirical Investigations of Our Model

In this chapter, we compare our approach with other recognised methods including conventional and modified perturbation theory. Then, we test our model on phenomenologically estimated data for a fit-invariant characteristic integral depending solely on the IR behaviour of the coupling constant.

3.1 Threshold Matching

In this section, we shall discuss the method we use for determining the values of $\Lambda^{(n_f)}$ to be employed in our calculation. For sufficiently large values of Q^2, our expression for the coupling constant reduces to the familiar one-loop formula $\alpha^{(1)}_{\mathrm{PT}}(Q^2)$. This suggests that our $\Lambda^{(n_f)}$ must coincide with the usual QCD scale parameter $\Lambda^{(n_f)}_{\mathrm{PT}}$ in momentum intervals corresponding to $n_f \geq 5$. Hence, we set our 5-flavour mass parameter $\Lambda^{(5)}$ equal to $\Lambda^{(5)}_{\mathrm{PT}}$ at the energy scale of the Z-boson mass $\mathrm{M}_Z = 91.19$ GeV. We extract the value $\Lambda^{(5)} = 0.135$ GeV from $\alpha^{(1)}_{\mathrm{PT}}(\mathrm{M}^2_Z)$ by means of the recent parametrisation of the hadronic decay width of the Z-boson [32]:

$$R_Z = 19.934 \left[1 + \sum_{k=1}^{n} a_k \left(\frac{\alpha^{(n)}_{\mathrm{PT}}(\mathrm{M}^2_Z)}{\pi} \right)^k \right], \tag{3.1}$$

where $n \leq 3$ denotes the n^{th} loop order under consideration, $a_1 = 1.045$, $a_2 = 0.94$, $a_3 = -15$ and $R_Z = 20.768$ [33]. To obtain the values of $\Lambda^{(4)}$ and $\Lambda^{(3)}$, which may differ from $\Lambda^{(4)}_{\rm PT}$ and $\Lambda^{(3)}_{\rm PT}$ as they correspond to lower energy intervals, we use the familiar threshold matching condition [36]:

$$\bar{\alpha}^{(1)}(Q_{th}; n_f) = \bar{\alpha}^{(1)}(Q_{th}; n_f - 1)\,, \tag{3.2}$$

at the energy thresholds $Q_{th} = 2\,m_b$ and $Q_{th} = 2\,m_c$, where $m_b = 4.21$ GeV and $m_c = 1.35$ GeV are the bottom- and charm-quark masses [22] respectively. In this way, starting with $\Lambda^{(5)} = 0.135$ GeV, we get $\Lambda^{(4)} = 0.188$ GeV and $\Lambda^{(3)} = 0.229$ GeV.

At light quark thresholds $Q_{th} \leq 2\,m_s$, where $m_s = 0.199$ GeV is the strange-quark mass [22], the applied matching condition (3.2) holds only approximately. This is also true for the analytic perturbation theory of Shirkov and Solovtsov [19]. For simplicity, instead of introducing a nontrivial and more complicated matching procedure such as the one used in Ref. [34], we choose to take $\Lambda^{(n_f)} = \Lambda^{(3)}$ for all $n_f \leq 3$. This choice is quite reasonable since it leads to:

$$\frac{\bar{\alpha}^{(1)}(Q_{th}; n_f)}{\bar{\alpha}^{(1)}(Q_{th}; n_f - 1)} \cong 1\,, \tag{3.3}$$

for all energy thresholds corresponding to $n_f < 3$. Furthermore, it is also supported by the good agreement with the value $\Lambda^{(0)} = 0.238\,(0.019)$ GeV obtained from quenched lattice QCD in Ref. [35].

3.2 Illustrative comparison

We begin by considering a quick comparison between the predictions in our approach and those in perturbation theory at one-, two- and three-loop order. Fig.(3.1) shows the behaviour of the 3-flavour running coupling $\bar{\alpha}^{(1)}(Q^2)$ together with $\alpha^{(1)}_{\rm PT}(Q^2)$, $\alpha^{(2)}_{\rm PT}(Q^2)$ and $\alpha^{(3)}_{\rm PT}(Q^2)$ in the low UV region as well as the Q-dependence of $\bar{\alpha}^{(1)}(Q^2)$ outside the perturbative domain. In this plot we use the same Λ values employed in Fig.(2.8) and take $\Lambda^{(3)} = 0.229$ GeV for our formula $\bar{\alpha}^{(1)}(Q^2)$. As is seen from Fig.(3.1.b), our model improves significantly on the 1-loop perturbative predictions and agrees well with the higher-loop estimates throughout the range $Q > 1.5$ GeV. In Fig.(3.1.a), we observe that the evolution of $\bar{\alpha}^{(1)}(Q^2)$ slows down appreciably as Q enters the IR region, $Q \leq \Lambda^{(3)}$,

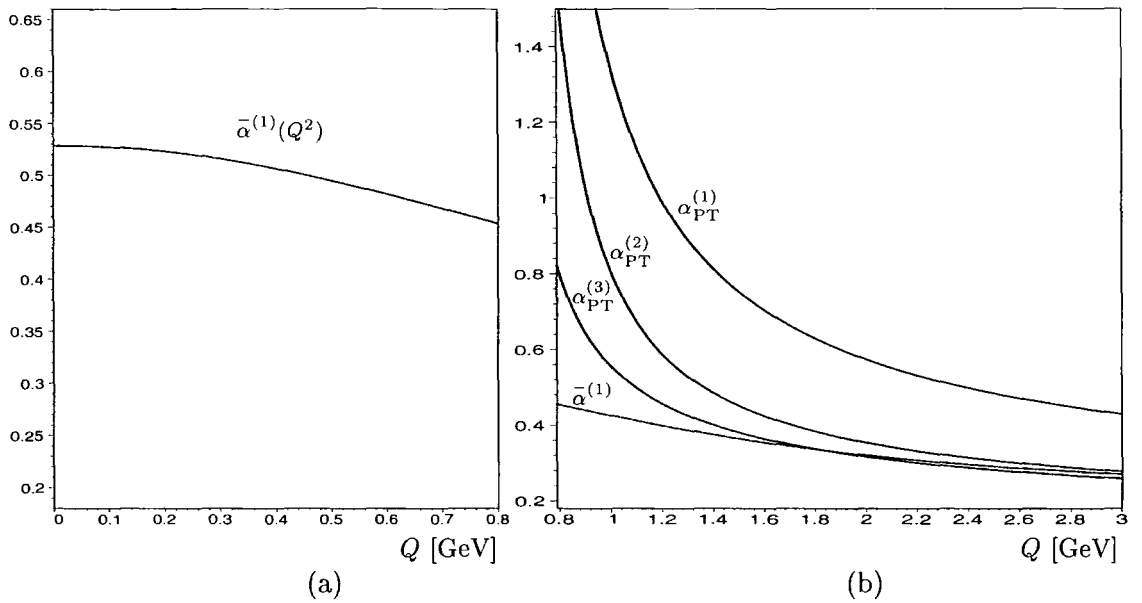


Figure 3.1: The IR freezing behaviour of our model (a) and a comparison of our model with the 1-, 2- and 3-loop perturbative expressions (b).

and freezes rapidly to a constant value of 0.529. This provides some direct theoretical evidence for the freezing of the running coupling at low energies, an idea that has long been a popular and successful phenomenological hypothesis. Phenomenological studies, such as [22] and references therein, show that a running coupling that freezes at low energies can be useful in describing experimental data and some IR effects in QCD. In the low energy domain: 0.8 GeV $\leq Q \leq$ 1.2 GeV , Badalian and Morgunov [37] extracted the value of the strong coupling constant $\alpha_s(Q^2)$ from the fits to charmonium spectrum and fine structure splittings. They found that $\alpha_s(Q^2) = 0.38 \pm 0.03(exp.) \pm 0.04(theory)$. This agrees reasonably well with our prediction, $\bar{\alpha}^{(1)}(Q^2) = 0.42 \pm 0.03$ in the same energy interval.

Within the 3-loop approximation of the optimized perturbation theory, Mattingly and Stevenson [22] found that the 2-flavour QCD running coupling α_s freezes below 0.3 GeV to a constant value of about 0.26 π. Although this value is quantitatively uncertain (while qualitatively unequivocal), it is not far off from our 1-loop prediction of 0.16 π.

A good theoretical approach which supports the IR freezing behaviour of our model follows from the work of Simonov and Badalian [14,15]. They studied the non-perturbative contributions to the QCD coupling constant on the basis of a new background field formalism, exploiting non-perturbative background correlation functions as a dynamical input.

In this framework, the one- and two-loop running coupling constants [15]:

$$\alpha_B^{(1)}(Q^2) = \frac{4\pi}{\beta_0}\frac{1}{\ln[(Q^2+M_B^2)/\Lambda_B^2]}, \tag{3.4}$$

$$\alpha_B^{(2)}(Q^2) = \frac{4\pi}{\beta_0}\frac{1}{\ln[(Q^2+M_B^2)/\Lambda_B^2]}\left[1-\frac{\beta_1}{\beta_0^2}\frac{\ln[\ln[(Q^2+M_B^2)/\Lambda_B^2]]}{\ln[(Q^2+M_B^2)/\Lambda_B^2]}\right], \tag{3.5}$$

were found to depend on a new parameter M_B (similar to λ_e in our model) known as the background mass. From a fit to the charmonium fine structure [37], it was found that $M_B = 1.1$ GeV. In Table(3.1), we list the values of $\Lambda_B^{(n_f)}$ for $n_f \leq 5$ in leading order (LO) and next-to-leading order (NLO). They are obtained as described in Ref. [15], using $\Lambda_{\rm PT}^{(5)} = 0.135$ GeV in LO and $\Lambda_{\rm PT}^{(5)} = 0.274$ GeV in NLO, which is basically the same method that we used to obtain the values of our $\Lambda^{(n_f)}$.

n_f	0	1	2	3	4	5
$\Lambda_B^{(n_f)}$ GeV LO	0.307	0.283	0.258	0.230	0.188	0.135
$\Lambda_B^{(n_f)}$ GeV NLO	0.569	0.553	0.535	0.509	0.414	0.274

Table 3.1: The values of $\Lambda_B^{(n_f)}$ in LO and NLO

In Fig.(3.2), we display the comparison between the 3-flavour coupling constant in our approach and those in the new background field formalism calculated to leading and next-to-leading order. As shown in the figure, our low energy estimates lie approximately in the middle between the predictions of $\alpha_B^{(1)}(Q^2)$ and $\alpha_B^{(2)}(Q^2)$, indicating the self-consistency of our results.

At the origin $Q = 0$, our results differ from that obtained by Shirkov and Solovtsov [19] by a small multiplicative factor $\kappa_e^{-1} = 0.38$, i.e. $\bar{\alpha}^{(1)}(0) = 0.38\ \alpha_{\rm an}^{(1)}(0)$, on the other hand we find that the estimates of the background coupling constants $\alpha_B^{(1)}(0)$ and $\alpha_B^{(2)}(0)$ are much closer to our predictions than to $\alpha_{\rm an}^{(1)}(0)$. Table(3.2) lists our results for $\bar{\alpha}^{(1)}(0)$ together with $\alpha_{\rm an}^{(1)}(0)$, $\alpha_B^{(1)}(0)$ and $\alpha_B^{(2)}(0)$ for $0 \leq n_f \leq 5$. The numerical value of our coupling constant $\bar{\alpha}^{(1)}(Q^2)$, as shown in table(3.2), is reasonably small which supports the notion of an expansion in powers of $\bar{\alpha}^{(1)}$ at low momentum transfers. Phenomenological verification of this fact would be of large practical value. Gribov's theory of confinement

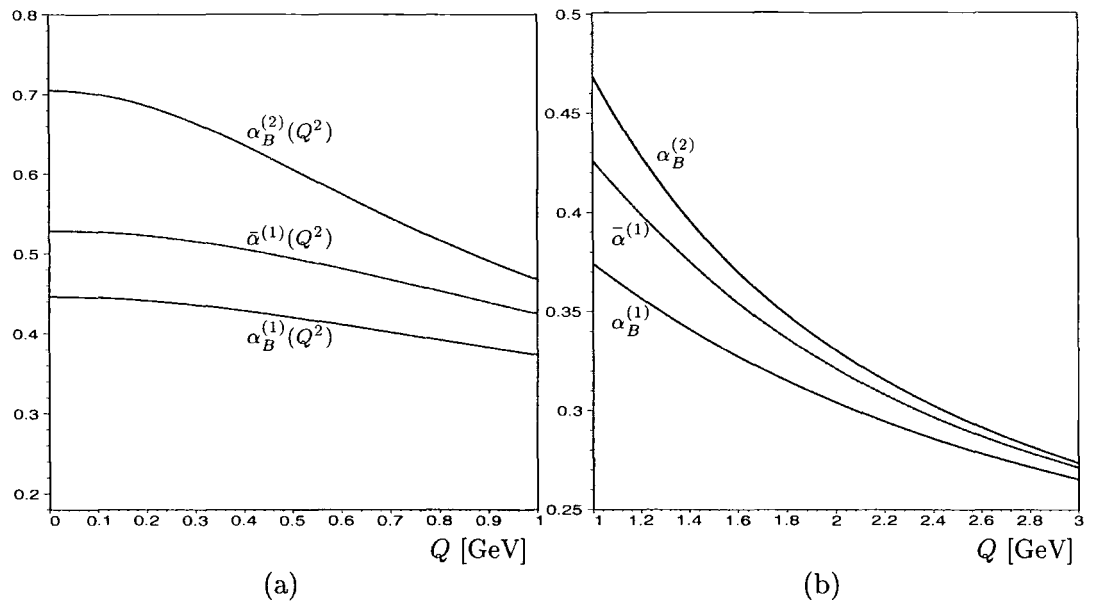


Figure 3.2: Illustrative comparison of our formula $\bar{\alpha}^{(1)}(Q)$ with the LO and NLO expressions for the background coupling constants $\alpha_B^{(1)}(Q)$ and $\alpha_B^{(2)}(Q)$ for $n_f = 3$.

n_f	0	1	2	3	4	5
$\bar{\alpha}^{(1)}(0)$	0.432	0.460	0.492	0.529	0.571	0.620
$\alpha_{\rm an}^{(1)}(0)$	1.142	1.216	1.300	1.396	1.508	1.639
$\alpha_B^{(1)}(0)$	0.448	0.448	0.448	0.446	0.427	0.391
$\alpha_B^{(2)}(0)$	0.713	0.713	0.714	0.705	0.576	0.447

Table 3.2: The values of $\bar{\alpha}^{(1)}(0)$ compared to those of $\alpha_{\rm an}^{(1)}(0)$, $\alpha_B^{(1)}(0)$ and $\alpha_B^{(2)}(0)$

[25] demonstrates how colour confinement can be achieved in a field theory of light fermions interacting with comparatively small effective coupling, a fact of potentially great impact for enlarging the domain of applicability of perturbative ideology to the physics of hadrons and their interactions [20].

In a number of cases of the QCD calculations it is necessary to estimate integrals of the form [38, 39]:

$$F(Q^2) = \int_0^Q \alpha_s(k^2)\, \mathrm{f}(k)\, dk\,, \tag{3.6}$$

where $\mathrm{f}(k)$ is a smooth function behaving like k^p at $k \ll Q$. In this integral, the interval of integration includes the IR region where the perturbative expression for the running coupling $\alpha_s(k^2)$ is inapplicable. Hence, by introducing an IR matching scale μ_I such that $\Lambda \ll \mu_I \ll Q$ the contribution to integral (3.6) from the region $k > \mu_I$ can be calculated

perturbatively. On the other hand, the portion of the integral below μ_I is expressed in Ref. [38] in terms of a non-perturbative parameter $\bar{\alpha}_p(\mu_I)$ as:

$$\int_0^{\mu_I} \alpha_s(k^2)\, k^p\, dk = \frac{\mu_I^{p+1}}{p+1}\, \bar{\alpha}_p(\mu_I) \tag{3.7}$$

For $\mu_I = 2$ GeV and $p = 0$, an excellent fit to experimental data yields: $A(2\,\mathrm{GeV}) = \bar{\alpha}_0(2\,\mathrm{GeV})/\pi = 0.18 \pm 0.03$ [20] and $A(2\,\mathrm{GeV}) = 0.17 \pm 0.01$ [38]. These results agree reasonably well with our estimate for $A(2\,\mathrm{GeV})$, which is obtained from (3.7) by direct substitution of our 3-flavour formula (2.74) for $\alpha_s(k^2)$, giving:

$$A(2\,\mathrm{GeV}) = \frac{2}{9}\int_0^2 \frac{1}{\ln(k^2/\Lambda^2) + E_1(\lambda_e\, k^2/\Lambda^2)}\, dk \;\cong 0.14\,. \tag{3.8}$$

Here $\lambda_e = 0.04$ and $\Lambda = 0.229$ GeV.

3.3 Gluon condensate

In QCD instantons are the best studied non-perturbative effects, leading to the formation of the gluon condensate, an important physical quantity defined as [43]:

$$K = \langle 0|\frac{\alpha_s}{\pi}\, F^a_{\mu\nu} F^a_{\mu\nu}|0\rangle\,, \tag{3.9}$$

where $F^a_{\mu\nu}$ is the Euclidean gluon field strength tensor and α_s is the quark-gluon coupling constant. This can be related to the total vacuum energy density ϵ_t of QCD by means of the famous trace anomaly relation [40, 41]:

$$\theta_{\mu\mu} = -\frac{\beta_0\, \alpha_s}{8\,\pi}\, F^a_{\mu\nu} F^a_{\mu\nu} + \sum_{f=1}^{n_f} m_f\, \overline{\Psi}_f\, \Psi_f + O(\alpha_s^2)\,, \tag{3.10}$$

where m_f and Ψ_f denote the quark masses and spinor quark fields respectively. Sandwiching $\theta_{\mu\mu}$ between the QCD vacuum states in the chiral limit (i.e. $m_f = 0$) and on account of the relation $\langle 0|\theta_{\mu\mu}|0\rangle = 4\,\epsilon_t$, see refs. [40, 43], one obtains:

$$K = -\frac{32}{\beta_0}\, \epsilon_t\,. \tag{3.11}$$

In the dilute instanton-gas approximation with $n_f = 0$, a direct relation between the gluon condensate K and the instanton density [42, 43]:

$$\rho(r) = \mathrm{b}\left[\frac{2\pi}{\alpha^{(1)}_{\mathrm{PT}}(r^{-2})}\right]^6 \exp\left(-\frac{2\pi}{\alpha^{(1)}_{\mathrm{PT}}(r^{-2})}\right), \tag{3.12}$$

with $r \approx 1/Q$ as the instanton scale size variable and $\mathrm{b} = 0.0015$ [42], can be represented in the form [43]:

$$K = 16 \int_0^{\mathrm{R_c}} \frac{\rho(r)}{r^5}\, dr\,, \tag{3.13}$$

where $\mathrm{R_c}$ is a cut-off introduced by hand to avoid the uncontrollable IR divergences. Since our formula for the running coupling (2.74) agrees reasonably well with the estimate of $\alpha^{(1)}_{\mathrm{PT}}$ at short distances $r < \mathrm{R_c}$ and is analytic for all $r \geq 0$, it is very tempting to use it in place of $\alpha^{(1)}_{\mathrm{PT}}$ to evaluate the integral in (3.13) in the limit $\mathrm{R_c} \to \infty$. If we do this, we arrive at:

$$K = 0.25 \times 11^6\, b\, \Lambda^4 \int_0^{\infty} x^6\, [\ln(x^{-2}) + E_1(\lambda_e\, x^{-2})]^6 \exp[-\frac{11}{2} E_1(\lambda_e\, x^{-2})]\, dx\,. \tag{3.14}$$

Here Λ corresponds to $n_f = 0$. A direct numerical integration of (3.14) yields:

$$K = 4.8624\ \Lambda^4\,. \tag{3.15}$$

Using the value $\Lambda = 0.229$ GeV, which we computed in section (3.1) for small n_f, we estimate the gluon condensate from (3.15) as $K = 0.013$ GeV^4. This is in good agreement with the value phenomenologically estimated from the QCD sum rules approach [43], namely $\langle 0|\frac{\alpha_s}{\pi}\, G^a_{\mu\nu} G^a_{\mu\nu}|0\rangle = 0.012$ GeV^4. In addition, our estimate for the gluon condensate is also consistent with that calculated phenomenologically in Ref. [44] and found to be $K = 0.014^{+0.0044}_{-0.0018}$ GeV^4. Note that if we had considered the value $\Lambda^{(0)} = 0.238$ GeV, obtained from quenched lattice QCD in Ref. [35], instead of our estimated value of Λ, we would have then found K to be 0.015 GeV^4, which is still close enough to the two phenomenological estimates mentioned above. Hence, it may well follow that the instanton density $\rho(r)$ is more likely to reveal more realistic and useful information when expressed in terms of our coupling constant $\bar{\alpha}^{(1)}$.

In Fig.(3.3), we shed some light on the dependence of $\rho(r)$ on the running couplings

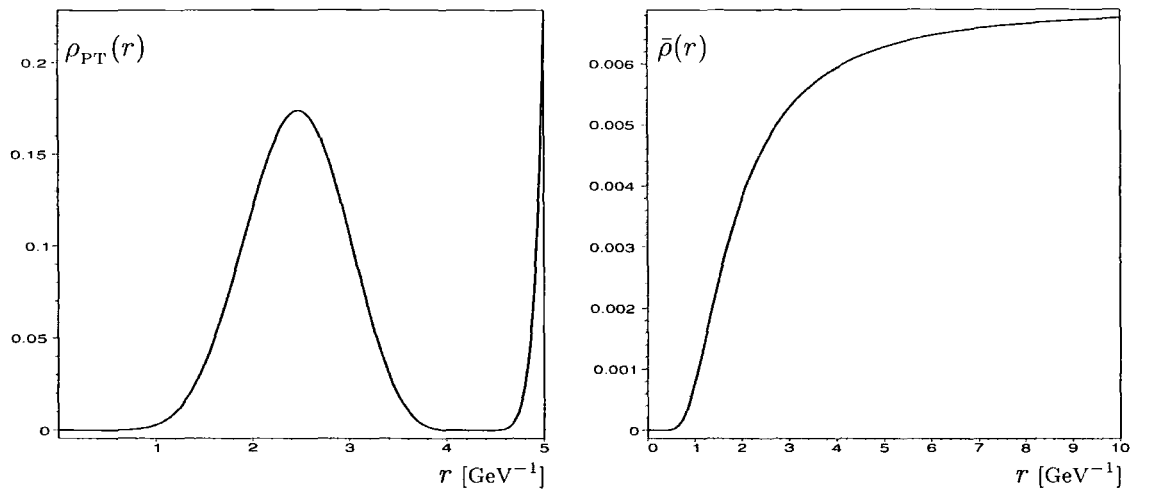


Figure 3.3: The behaviour of the instanton density as expressed in terms of the running couplings (a) $\alpha_{PT}^{(1)}$, and (b) $\bar{\alpha}^{(1)}$.

$\alpha_{PT}^{(1)}$ and $\bar{\alpha}^{(1)}$ which we shall denote by $\rho_{PT}(r)$ and $\bar{\rho}(r)$ respectively. As seen in Fig.(3.3), at short distances, say $r < 0.6$ GeV^{-1}, $\rho_{PT}(r)$ and $\bar{\rho}(r)$ agree reasonably well whereas when we increase r to sufficiently larger values $\rho_{PT}(r)$ rises very rapidly towards infinity while $\bar{\rho}(r)$ stabilizes to a fixed density. This reflects the practical usefulness of our approach to the strong coupling constant.

3.4 QCD β–function and IR properties

In quantum chromodynamics, the β–function in the renormalisation group (RG) equation:

$$\beta(\alpha(Q^2)) = Q^2 \frac{d\,\alpha(Q^2)}{dQ^2}, \tag{3.16}$$

has the perturbative expansion [45]:

$$\beta(\alpha) = -\alpha \sum_{n=0}^{\infty} \beta_n \left(\frac{\alpha}{4\pi}\right)^{n+1}, \tag{3.17}$$

where β_0, β_1 and β_2 are given by (1.166), (2.66) and (2.67) respectively and [46]:

$$\beta_3 = 29243.0 - 6946.30\,n_f + 405.089\,n_f^2 + 1.49931\,n_f^3. \tag{3.18}$$

Here the higher-order coefficients β_n for $n > 3$ have not been calculated till now. Generally speaking, (3.16) is the crucial equation that decides whether or not there is a so-called stable fixed point at the origin (i.e. whether $\beta(\alpha) = 0$ for $\alpha = 0$) of either the infrared or ultraviolet type, with implications for the absence or presence of asymptotic freedom in the gauge theory under consideration. The distinction between an infrared and an ultraviolet stable fixed point depends on whether the derivative $\beta'(\alpha) > 0$ or $\beta'(\alpha) < 0$ at $\alpha = 0$ respectively. In both kinds of gauge theories (Abelian and non-Abelian), there is a stable fixed point at the origin but it turns out that, while $\beta'(\alpha) > 0$ (stable IR fixed point) for an Abelian gauge theory, the reverse is true for a non-Abelian gauge theory , i.e. $\beta'(\alpha) < 0$ (stable UV fixed point). In general, it is extremely difficult to establish the existence of stable fixed points of a quantum field theory of $\beta(\alpha)$ for $\alpha \neq 0$ [47]. In perturbative QCD, the one-, two-, three- and four-loop $\beta-$function with quark flavours $n_f \leq 6$ fail to exhibit any non-trivial zero that can be interpreted as a stable IR fixed point. Because of this, the perturbative QCD coupling constant $\alpha_{\rm PT}(Q^2)$ blows up as $Q^2 \to 0$.

Our main task in this section is to demonstrate how the $\beta-$function in our approach can provide useful information about the IR region that a truncated perturbative series can not. As a cross check on our method, we shall calculate the stable IR fixed point for any number of quark flavour and show that it is consistent with our previous result (2.76). Starting from (2.74) with $\bar{\alpha}^{(1)}$ being renamed as α, our QCD $\beta-$function in accordance with the definition (3.16) assumes the form:

$$\bar{\beta}(\alpha) = -\frac{\beta_0}{4\,\pi}\,\alpha^2\,[1 - {\rm e}^{-\Omega(\alpha)}]\,, \tag{3.19}$$

where

$$\Omega(\alpha) = {\rm e}^{\phi(\alpha)}\,, \tag{3.20}$$

and the function $\phi(\alpha)$ is defined by the transcendental relation:

$$\phi(\alpha) + E_1({\rm e}^{\phi(\alpha)}) = \frac{4\,\pi}{\beta_0\,\alpha} + \ln(\lambda_e)\,. \tag{3.21}$$

In the following domains of α:

$$D_1 = \{\,\alpha : \phi(\alpha) \geq 3\,\} = \{\,\alpha : 0 < \alpha \leq 2.021\,\beta_0^{-1}\,\}\,, \tag{3.22}$$

and

$$D_2 = \{\, \alpha : \phi(\alpha) \leq -4 \,\} = \{\, \alpha :\ 4.724\,\beta_0^{-1} \leq \alpha < 4.757\,\beta_0^{-1} \,\}\,, \tag{3.23}$$

a good approximate solution of (3.21) can be found as:

$$\phi(\alpha) \cong \begin{cases} \dfrac{4\pi}{\beta_0\alpha} + \ln(\lambda_e) - E_1(\lambda_e \exp\left(\dfrac{4\pi}{\beta_0\alpha}\right)) & \text{if } \alpha \in D_1, \\ \\ \ln\left(\dfrac{4\pi}{\beta_0\alpha} - \kappa_e\right) & \text{if } \alpha \in D_2. \end{cases} \tag{3.24}$$

We note that as α approaches zero, $\phi(\alpha)$ grows without limit, allowing (3.19) to reproduce the conventional one-loop QCD $\beta-$function. It follows from (3.19) that for all n_f satisfying $\beta_0(n_f) > 0$ there exists a stable IR fixed point $\alpha_{\rm FP}$ identified by $\Omega(\alpha_{\rm FP}) = 0$. Using the expansion of (2.21) in (3.21), we obtain, in the limit $\Omega(\alpha) \to 0$, the function:

$$\Omega(\alpha) = \frac{4\pi}{\beta_0\alpha} - \kappa_e\,, \tag{3.25}$$

from which $\alpha_{\rm FP}$ is found to be:

$$\alpha_{\rm FP} = \frac{4\pi}{\beta_0\,\kappa_e}\,. \tag{3.26}$$

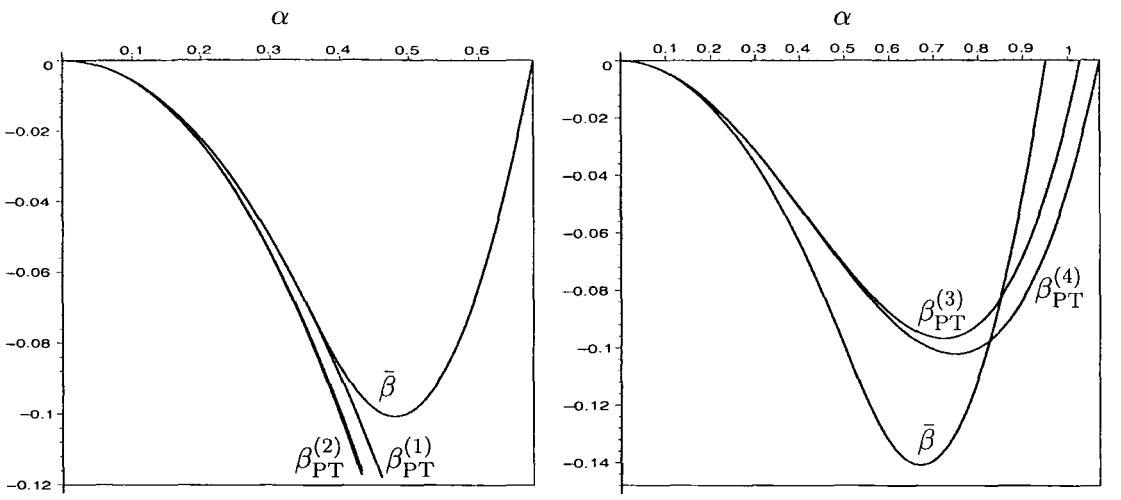
This is completely consistent, as it should be, with our previous result (2.76).

For $6 < n_f \leq 16$, the higher-order terms of the QCD $\beta-$function are known to permit the occurrence of IR fixed points. For example, for all values of n_f such that $\beta_0(n_f) > 0$ and $\beta_1(n_f) < 0$ the two-loop $\beta-$function $\beta^{(2)}_{\rm PT}(\alpha)$ [1] possesses a non-trivial IR fixed point given by:

$$\alpha^{(2)}_{\rm FP} = -\frac{4\pi\,\beta_0}{\beta_1} > 0\,. \tag{3.27}$$

This may sound fine. However, the IR fixed points arising from the truncation of the perturbative series (3.17) are likely to be spurious. For instance, at the candidate value for $\alpha_{\rm FP}$, the first and second order terms in $\beta^{(2)}_{\rm PT}(\alpha)$ are equal in magnitude (i.e. $|\beta_0\,\alpha^{(2)^2}_{\rm FP}/4\pi| = |\beta_1\,\alpha^{(2)^3}_{\rm FP}/(4\pi)^2|$), indicating the inefficiency of the two-loop approximation around the calculated IR fixed point (3.27). In fact, there is no way to prove that the IR fixed points ex-

[1] The notations $\beta^{(n)}_{\rm PT}(\alpha)$ and $\alpha^{(n)}_{\rm FP}$ are used to denote the n-loop $\beta-$function and its corresponding IR fixed point respectively.



(a) (b)

Figure 3.4: The behaviour of the β–function in our approach and in perturbation theory for $n_f = 6$ (a) and $n_f = 9$ (b). In (a), the curves of $\beta^{(2)}_{\rm PT}(\alpha)$, $\beta^{(3)}_{\rm PT}(\alpha)$ and $\beta^{(4)}_{\rm PT}(\alpha)$ coincide and none of them achieves a perturbative IR fixed point. In (b), the locations of the fixed points are different but very close to each other.

tracted from perturbation theory alone are indeed the positive zeros of the true β–function or anywhere near them. However, it is still worthwhile to test the perturbative expansion (3.17) to 4-loop order against our model for the β–function. In Fig.(3.4), we demonstrate the full behaviour of our β–function together with its perturbative counterpart for $n_f = 6$ and 9. As seen in the figure, the β–function in our approach $\bar{\beta}(\alpha)$ agrees very well with the correct perturbative predictions at and near the UV fixed point $\alpha = 0$. As α leaves the region D, where $D = \{\alpha : 0 \leq \alpha \leq 2.7/\beta_0(n_f)\}$, $\bar{\beta}(\alpha)$ starts to diverge significantly from $\beta^{(1)}_{\rm PT}(\alpha)$ and changes direction, turning back to zero in the limit $\alpha \to \alpha_{\rm FP}$ as depicted in Fig.(3.4.a) for $n_f = 6$. The occurrence of IR fixed points in $\beta^{(2)}_{\rm PT}(\alpha)$, $\beta^{(3)}_{\rm PT}(\alpha)$ and $\beta^{(4)}_{\rm PT}(\alpha)$ takes place only if $n_f \in [9,16], [7,16]$ and [8,16] respectively. In these n_f–intervals, we find that the two-, three- and four-loop β–functions behave qualitatively like $\bar{\beta}(\alpha)$. This is illustrated in Fig.(3.4.b) with $\beta^{(3)}_{\rm PT}(\alpha)$ and $\beta^{(4)}_{\rm PT}(\alpha)$ for $n_f = 9$. It would have been interesting to see whether this qualitatively similar behaviour continues beyond the 4-loop order. Unfortunately, we know of no existing argument or calculation that definitively answers this question.

In table(3.3), we list the values of the IR fixed points in our approach and those allowed in perturbation theory within the two-, three- and four-loop approximations for $6 < n_f < 16$. For $n_f \in [8,16]$, the four-loop β–function $\beta^{(4)}_{\rm PT}$ has two positive roots.

n_f	7	8	9	10	11	12	13	14	15
$\alpha_{\rm FP}$	0.751	0.839	0.951	1.098	1.297	1.586	2.039	2.854	4.757
$\alpha^{(2)}_{\rm FP}$	*	*	5.236	2.208	1.234	0.754	0.468	0.278	0.143
$\alpha^{(3)}_{\rm FP}$	2.457	1.464	1.028	0.764	0.579	0.435	0.317	0.215	0.123
$\alpha^{(4)}_{\rm FP}$	*	1.550	1.072	0.815	0.626	0.470	0.337	0.224	0.126
$\alpha^{(4)}_{\rm UVFP}$	*	14.364	12.090	5.617	3.294	2.295	1.781	1.480	1.286

Table 3.3: The values of $\alpha_{\rm FP}$ compared to those of $\alpha^{(2)}_{\rm FP}$, $\alpha^{(3)}_{\rm FP}$ and $\alpha^{(4)}_{\rm FP}$. The * sign denotes the non-existence of a positive fixed point.

The smaller of these is an IR fixed point whereas the larger one is an UV fixed point. Thus, we shall denote the latter by $\alpha^{(4)}_{\rm UVFP}$. From table(4.1), we find that with increasing n_f our IR fixed point $\alpha_{\rm FP}$ increases gradually whereas the perturbative roots $\alpha^{(2)}_{\rm FP}$, $\alpha^{(3)}_{\rm FP}$, $\alpha^{(4)}_{\rm FP}$ and $\alpha^{(4)}_{\rm UVFP}$ decrease to smaller values. However, for most values of n_f we observe that the further $\alpha_{\rm FP}$ is from one root of some order, say $\alpha^{(n)}_{\rm FP}$, the closer it is to another root of different order, say $\alpha^{(n\pm1)}_{\rm FP}$. For example, for any $n_f \in [8,10]$ we find $\alpha_{\rm FP}$ to be closer in magnitude to $\alpha^{(3)}_{\rm FP}$ and $\alpha^{(4)}_{\rm FP}$ than to $\alpha^{(2)}_{\rm FP}$ and $\alpha^{(4)}_{\rm UVFP}$. On the other hand, for any $n_f \in [12,14]$ our estimate for $\alpha_{\rm FP}$ is much closer to $\alpha^{(4)}_{\rm UVFP}$ than to any other value of the perturbative IR fixed points. Also, for $n_f = 11$ we have $\alpha_{\rm FP} \approx \alpha^{(2)}_{\rm FP}$. This analysis may not be conclusive however it provides us with some element of truth about our estimate for the possible magnitude of the true IR fixed point.

It is noteworthy that (3.26) enables us to express λ_e in terms of $\alpha_{\rm FP}$ as:

$$\lambda_e = \exp\left(-\gamma - \frac{4\pi}{\beta_0\,\alpha_{\rm FP}}\right). \tag{3.28}$$

This could have a direct beneficial effect on our approach if accurate phenomenological estimates for the IR fixed points were available. Indeed, if this were the case (3.28) would allow us to determine the only free parameter, λ_e, in the theory straightforwardly. However, in the absence of this phenomenological data, the method we used in obtaining the value $\lambda_e = 0.04$ remains an adequate alternative as it results in a good approximation for the QCD β–function with any number of quark flavours.

Chapter 4

Exact Two-Loop Calculation

In this chapter, we shall solve the RG equation (3.16) at the two-loop order, giving an exact solution for the running coupling $\alpha_{LW}^{(2)}(Q^2)$ expressed in terms of the so-called Lambert's W-function. Then, we study the analyticity structure of this solution. To remove the nonphysical singularities emerging from the two-loop approximation and to further investigate the IR behaviour of the QCD coupling constant without altering the correct UV properties, we apply our approach to the perturbative expression $\alpha_{LW}^{(2)}(Q^2)$ in the same way as described in chapter 2. In this way, we obtain a regular solution $\bar{\alpha}_{LW}^{(2)}(Q^2)$ that freezes to a constant value at the extreme IR limit $Q^2 = 0$.

4.1 Lambert's W-Function

In this section we shall give a concise review of the basic properties of the so-called Lambert's W-function, which plays an important role in solving the two-loop RG equation in QCD [17]. Lambert's W-function is a multivalued special function, defined as the solution $W(z)$ of the transcendental equation [48]:

$$W(z)\, \mathrm{e}^{W(z)} = z, \qquad z \in \mathbb{C}, \tag{4.1}$$

and has an infinite number of branches, each denoted by $W_n(z)$ with n being a branch index. For $x \in \mathbb{R}^+$, there is only one real branch of $W(x)$, but for $x \in [-1/\mathrm{e}, 0)$ there are two, namely $W_0(x)$ and $W_{-1}(x)$ as shown in Fig.(4.1). Following Ref. [48], we denote the branches satisfying $W(x) \geq -1$ and $W(x) \leq -1$ by $W_0(x)$ and $W_{-1}(x)$ respectively.

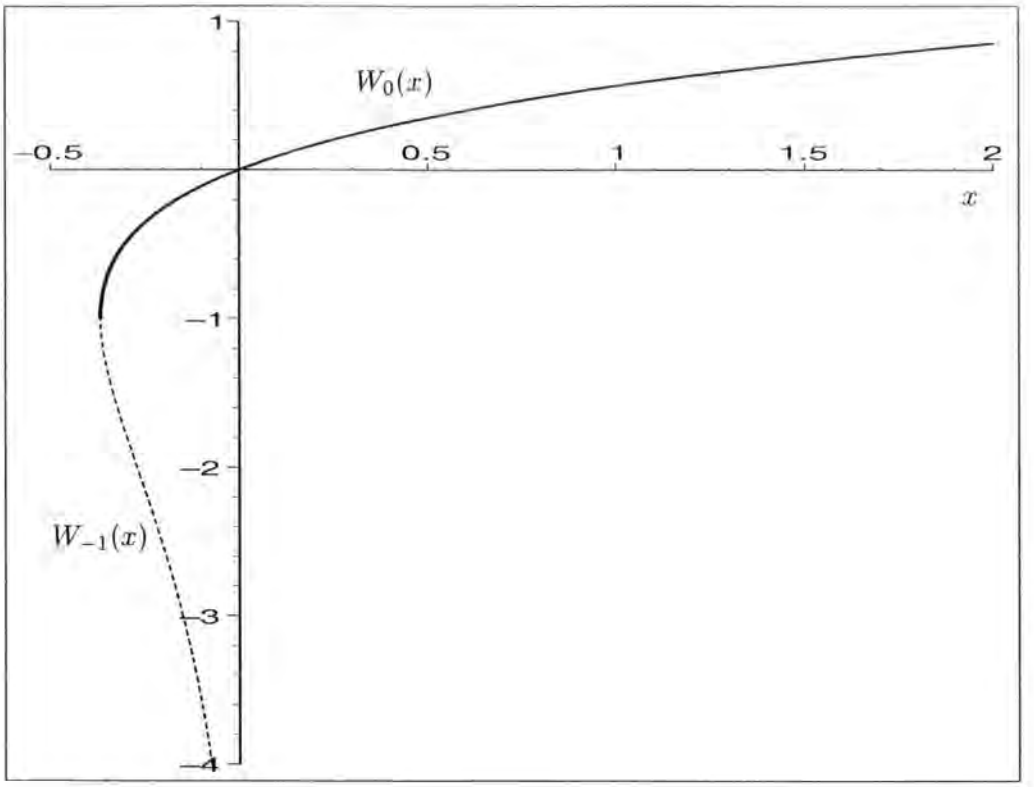


Figure 4.1: The two real branches of $W(x)$. The dashed and solid curves represent $W_{-1}(x)$ and $W_0(x)$ respectively.

$W_0(z)$ is referred to as the principal branch of Lambert's W-function. For $x > 0$, $W_0(x)$ and $W_{-1}(x)$ allow us to write the natural logarithm $\ln(x)$ as:

$$\ln(x) = \begin{cases} W_{-1}(x \ln(x)) & \text{if } x \in (0, 1/\mathrm{e}], \\ W_0(x \ln(x)) & \text{if } x \geq 1/\mathrm{e}. \end{cases} \tag{4.2}$$

From the definition of $W(x)$, Lémeray noted that as $x = W(a)$ is a solution of $x\,\mathrm{e}^x = a$ a variety of other equations can be solved in terms of the same transcendental function. For example, the solution of $x\,b^x = a$ is $x = W(a \ln(b))/\ln(b)$, the solution of $x^{x^a} = b$ is $\exp\{W(a \ln(b))/a\}$ and the solution of $a^x = x + b$ is $x = -b - W(-a^{-b} \ln(a))/\ln(a)$.

To obtain the first derivative of Lambert's W-function, we simply differentiate the defining equation (4.1) with respect to z and then solve for $W'(z)$. In this way, we arrive at:

$$W'(z) = \frac{W(z)}{z\,[\,1 + W(z)\,]}, \tag{4.3}$$

where $z = 0$ is not allowed for the non-principal branches. By taking further derivatives, we deduce by induction the following expression [48] for the nth derivative of W:

$$\frac{d^n W(z)}{dz^n} = \frac{\exp(-n\,W(z))\,P_n(W(z))}{[\,1 + W(z)\,]^{(2n-1)}} \qquad \text{for } n \geq 1\,, \tag{4.4}$$

where the polynomials $P_n(W)$ satisfy the recurrence relation:

$$P_{n+1}(W) = -(n\,W + 3n - 1)\,P_n(W) + (1 + W)\,P_n'(W) \qquad \text{for } n \geq 1\ . \tag{4.5}$$

Here, the initial polynomial is $P_1(W) = 1$ and the value of $P_n(W)$ for $W = 0$ is given by:

$$P_n(0) = \frac{(-n)^{n-1}}{n!} \qquad \text{for } n \geq 1\ . \tag{4.6}$$

We remark here that the principal branch $W_0(z)$ is the only branch which is infinitely differentiable at the origin. For example, given $W_0(0) = 0$ it follows from (4.4) that

$$\left.\frac{d\,W(z)}{dz}\right|_{z=0} = \left.\frac{\exp(-W(z))}{[\,1 + W(z)\,]}\right|_{z=0} = 1\,. \tag{4.7}$$

Hence, by use of (4.4), we can easily compute the following Maclaurin series expansion for $W_0(z)$:

$$W_0(z) = \sum_{n=1}^{\infty} \frac{(-n)^{n-1}}{n!}\,z^n\,, \tag{4.8}$$

where $|z| < 1/\mathrm{e}$ is the radius of convergence.

A detailed discussion of the complex branches of Lambert's W-function can be found in Ref. [48]. For clarity, however, we give here a brief overview of the description of these branches. Fig.(4.2) illustrates the complex range of the principal branch W_0 together with those of $W_{-1}(z)$ and $W_1(z)$. To specify the boundary curves for each branch W_n and to find the images of these boundaries on the complex $z-$plane, i.e. the branch cuts of all the branches of $W(z)$, we first separate the real and imaginary parts of (4.1) as:

$$\mathrm{Re}\,z \;=\; \mathrm{e}^{\xi}\,[\,\xi\,\cos(\eta) - \eta\,\sin(\eta)\,], \tag{4.9}$$

$$\mathrm{Im}\,z \;=\; \mathrm{e}^{\xi}\,[\,\eta\,\cos(\eta) + \xi\,\sin(\eta)\,], \tag{4.10}$$

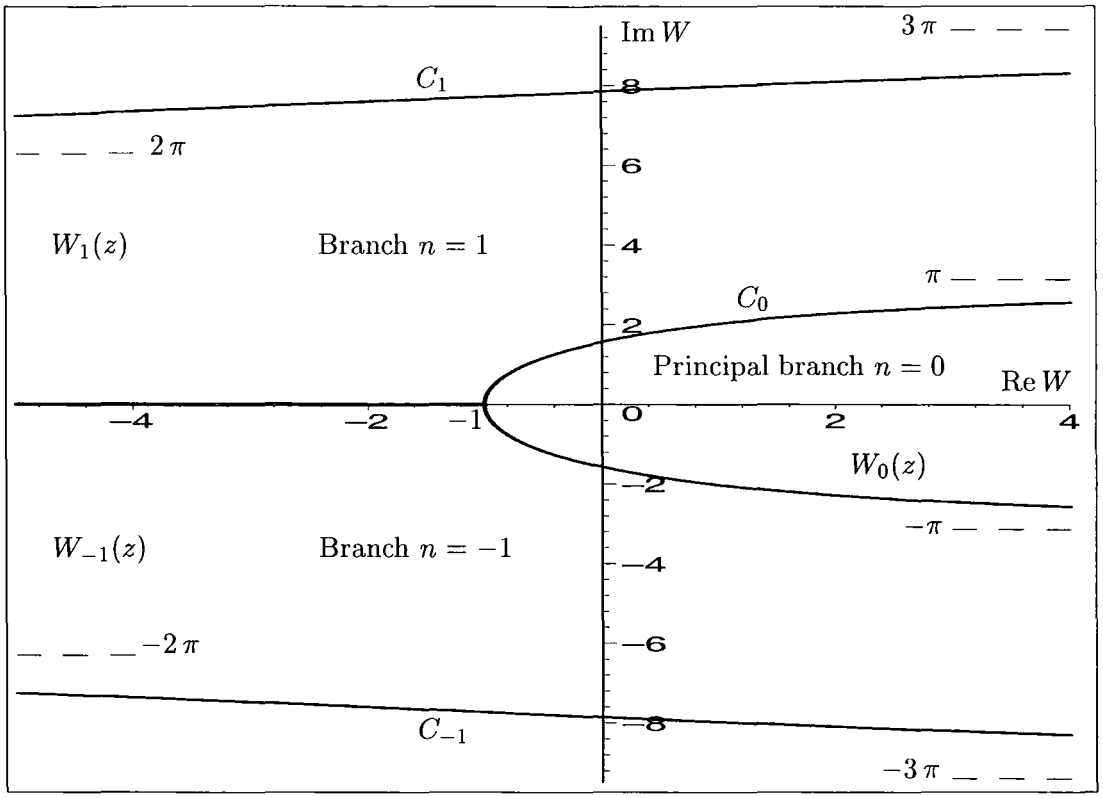


Figure 4.2: The ranges of the branches of $W(z)$. Each branch is given a number, the principal branch being numbered 0. The boundary curves C_n of the branches are asymptotic to the dashed lines, which are horizontal at multiples of $\pm\pi$.

where $\xi = \mathrm{Re}\, W$ and $\eta = \mathrm{Im}\, W$. Then, we define the boundary curves such that their images lie on the negative real axis of the $z-$plane, similar to the familiar choice of the branch cut of the complex logarithm. Therefore, If we let $\mathrm{Im}\, z = 0$ in (4.10), resulting in $\eta = 0$ or $\xi = -\eta \cot(\eta)$, and take $\xi \cos(\eta) - \eta \sin(\eta) < 0$ we obtain a set of curves that partition the $W-$plane into $n-$branches as shown in Fig.(4.2). The curve which separates the principal branch W_0 from the neighbouring branches W_1 and W_{-1} is given by:

$$C_0 = \{-\eta \cot(\eta) + i\,\eta : -\pi < \eta < \pi\} \tag{4.11}$$

and the curve that disconnects the adjacent branches W_1 and W_{-1} on the left-half plane $\mathrm{Re}\, W < 0$ is simply the line $(-\infty, -1]$, corresponding to $\mathrm{Im}\, z = 0$ and $\mathrm{Re}\, z \in [-1/\mathrm{e}, 0)$.

Finally, we write the set of curves C_n separating the remaining $n-$branches as:

$$C_n = \begin{cases} \{ -\eta \cot(\eta) + i\,\eta : 2n\,\pi < \eta < (2n+1)\,\pi \} & \text{for } n \geq 1, \\ \{ -\eta \cot(\eta) + i\,\eta : (2n-1)\,\pi < \eta < 2n\,\pi \} & \text{for } n \leq -1\ . \end{cases} \tag{4.12}$$

For all multivalued functions, the division of the complex plane into branches is somewhat arbitrary, and even the elementary functions do not have universally accepted branches. One of the benefits of our choice for placing the branch cut on the negative real axis is that it allows for the near conjugate symmetry:

$$W_n(z^*) = W_{-n}^*(z)\,, \qquad z = |z|\,\mathrm{e}^{i\arg(z)}\,, \tag{4.13}$$

for all integers n. As explained in Ref. [48], each $n-$partition W_n in the $W-$plane maps bijectively onto the $z-$plane. In Fig.(4.2), the points on each boundary C_n or $(-\infty, -1]$ belong to the branch below them, satisfying the counter-clockwise continuity [48]. For example, $W_1(z)$ contains no part of the real interval $(-\infty, -1]$ in its range whereas $W_{-1}(z)$ includes the whole of this interval in its range by choice of closure [48]. The principal branch $W_0(z)$ is the only analytic branch at $z = 0$ and also the only branch with a range including all positive real values. $W_0(z)$ has a branch point at $z = -1/\mathrm{e}$, corresponding to $W_0 = -1$, and a branch cut given by $\{z : -\infty < z \leq -1/\mathrm{e}\}$. The two branches $W_{-1}(z)$ and $W_1(z)$ both share the same branch points at $z = -1/\mathrm{e}$ and $z = 0$, and each of them has a double branch cut, $\{z : -\infty < z \leq -1/\mathrm{e}\}$ and $\{z : -\infty < z \leq 0\}$. On the other hand, all the other branches take the negative real axis $\mathrm{Re}\, z \leq 0$ and the origin $z = 0$ as their only branch cut and branch point respectively. Since the values of $W_n(z)$ along the branch cut are determined by the rule of counter-clockwise continuity around the branch point, $W_0(z)$ and $W_{-1}(z)$ are the only branches that can take on real values.

A useful asymptotic expansion for the non-principal branches of Lambert's W-function both at infinity and at zero is given by [48]:

$$\begin{aligned} W_n(z) &= \log(z) + 2\pi i\, n - \log[\log(z) + 2\pi i\, n] \\ &+ \sum_{l=0}^{\infty} \sum_{m=1}^{\infty} C_{lm}\, \frac{\log^m[\log(z) + 2\pi i\, n]}{[\log(z) + 2\pi i\, n]^{l+m}}\,, \end{aligned} \tag{4.14}$$

where $\log(z) = \ln|z| + i\arg(z)$, with $-\pi < \arg(z) \leq \pi$, and $C_{lm} = \frac{(-1)^l}{m!} \left[\begin{smallmatrix} l+m \\ l+1 \end{smallmatrix} \right]$ with $\left[\begin{smallmatrix} l+m \\ l+1 \end{smallmatrix} \right]$ being a Stirling cycle number [1] [49,50]. This expansion is absolutely convergent for large enough z and yields reasonably accurate results for $z \gtrsim 3$. For $W_{-1}(z)$, the above expansion (4.14) is not valid for z tending to 0 along the negative real axis, but holds otherwise. By a similar argument to that used in obtaining (4.14), Corless *et al* gave useful guidelines for finding a simple asymptotic expression for $W_{-1}(z)$ for sufficiently small and negative values of z:

$$W_{-1}(z) \approx \ln(-z) - \ln[\ln(-z)]\,. \tag{4.15}$$

As stated in Ref. [48], the complex logarithm of $W_n(z)$ satisfies the following relation:

$$\log W_n(z) = -W_n(z) + \psi_n(z)\,, \tag{4.16}$$

where

$$\psi_n(z) = \begin{cases} \log(z) & \text{if } n = -1 \text{ and } z \in [-1/\mathrm{e}\,,\, 0\,), \\ \log(z) + 2\pi i n & \text{otherwise.} \end{cases} \tag{4.17}$$

This, together with the fact that $\log W_n = \ln|W_n| + i\arg\{W_n\}$, gives:

$$\arg\{W_n(z)\} = \arg(z) + 2\pi n - \mathrm{Im}\{W_n(z)\} \tag{4.18}$$

unless $n = -1$ and $z \in [-1/\mathrm{e}\,,\, 0\,)$, in which case we have $\arg\{W_{-1}(z)\} = \pi$. It also follows that:

$$|W_n(z)| = |z|\mathrm{e}^{-\mathrm{Re}\{W_n(z)\}}\,. \tag{4.19}$$

For $\arg(z) = \pi$, we have that $\arg\{W_n(z)\} \to 0$ in the limit $|z| \to \infty$. The special case $\arg\{W_n(z)\} = 0$ implies $n = 0$ and z is real and positive. This follows from the

[1] Stirling cycle numbers $\left[\begin{smallmatrix} n \\ m \end{smallmatrix} \right]$ are defined by

$$\ln^m(1+z) = m! \sum_{n=m}^{\infty} (-1)^{n+m} \left[\begin{smallmatrix} n \\ m \end{smallmatrix} \right] \frac{z^n}{n!}\,,$$

where the numbers $(-1)^{n+m} \left[\begin{smallmatrix} n \\ m \end{smallmatrix} \right]$ are also called Stirling numbers of the first kind [50].

fact that $W_0(z)$ is the only branch which is real and positive for all $z \geq 0$. However, if $\arg\{W_n(z)\} = \pi$ then the branch index n can be 0 or -1, and for either case $z \in [-1/\mathrm{e}\,,\, 0\,)$.

For $z > 0$, it follows from (4.16) that the principal branch $W_0(z)$ satisfies the following relation:

$$W_0(z) = \ln(z) - \ln[W_0(z)]\,. \tag{4.20}$$

Solving this iteratively for $W_0(z)$, we obtain to one iteration a reasonable approximate solution for large positive z

$$W_0(z) \approx \ln(z) - \ln\ln(z)\,. \tag{4.21}$$

4.2 The exact 2-loop Lambert's W-solution

In this section, we shall show how to obtain an exact solution of the two-loop RG equation by using the definition of $W_n(z)$. This is perhaps the most significant use of Lambert's W-function in QCD. Starting with the two-loop RG equation:

$$\frac{d\,\alpha^{(2)}(Q^2)}{d\,\ln(Q^2)} = -\tilde{\beta}_0\,{\alpha^{(2)}}^2(Q^2)\left[1 + b\,\alpha^{(2)}(Q^2)\right], \tag{4.22}$$

where $\tilde{\beta}_0 = (4\pi)^{-1}\,\beta_0$ and $b = (4\pi\,\beta_0)^{-1}\,\beta_1$, we obtain by a straightforward integration:

$$-\frac{1}{\alpha^{(2)}(Q^2)} + b\,\ln\left|\frac{1}{\alpha^{(2)}(Q^2)} + b\right| + \tilde{\beta}_0\ln(Q^2) = \mathrm{C}\,, \tag{4.23}$$

with C being an arbitrary constant of integration. Note that when integrating (4.22), the values $\alpha^{(2)} = 0$ and $\alpha^{(2)} = -1/b$ have been excluded to avoid division by zero. For $b < 0$, (4.22) has an IR fixed point at $\alpha^{(2)} = 1/|b|$. In this case we shall be involved only with the range $\{\alpha^{(2)} : 0 < \alpha^{(2)} < 1/|b|\}$ because here the theory is asymptotically free. Hence, regardless of the sign of b, we may safely remove the absolute-value bars from the argument of the logarithm in (4.23). Now, taking [2]:

$$\mathrm{C} = \tilde{\beta}_0\,\ln\Lambda^2 + b\,\ln|b|\,, \tag{4.24}$$

[2]For consistency with the definition of Landau ghost-pole singularity in leading order, we take the constant C as in (4.24), locating the singularity in $\alpha^{(2)}(Q^2)$ at $Q^2 = \Lambda^2$.

gives:

$$\tilde{\beta}_0 \ln(Q^2/\Lambda^2) = \frac{1}{\alpha^{(2)}} - b \ln\left(\varepsilon(b) + \frac{1}{|b|\,\alpha^{(2)}}\right), \tag{4.25}$$

where $\varepsilon(b) = b/|b|$. Here, the QCD mass scale parameter Λ is different in magnitude from that in (1.165), but for simplicity we use the same notation throughout. At this stage, it is clear from (4.25) that $\alpha^{(2)}(Q^2)$ has a cut on the negative real axis, being a function of $\ln(Q^2/\Lambda^2)$. For small enough values of $\alpha^{(2)}$, the transcendental equation (4.25) can be solved approximately for $\alpha^{(2)}(Q^2)$, by the fixed-point iteration technique, giving up to one iteration:

$$\alpha_I^{(2)}(Q^2) = \frac{1}{\tilde{\beta}_0 \ln(Q^2/\Lambda^2) + b \ln\left(\varepsilon(b) + |b|^{-1} \ln(Q^2/\Lambda^2)\right)}. \tag{4.26}$$

From this formula, we can correctly reproduce the standard two-loop expression (2.64), denoted by $\alpha_{\rm PT}^{(2)}(Q^2)$. Although both expressions $\alpha_I^{(2)}(Q^2)$ and $\alpha_{\rm PT}^{(2)}(Q^2)$ give correct estimates at sufficiently large momenta, they are inadequate for studying the singularity structure of the exact solution $\alpha^{(2)}(Q^2)$ of (4.25). Moreover, they do not allow for the expected perturbative freezing when $b < 0$, because in these approximations the logarithmic terms become dominant in the IR region. Without using approximation methods, we now calculate $\alpha^{(2)}(Q^2)$ explicitly in terms of Lambert's W function. If we rewrite (4.25) as:

$$\ln\left(\frac{Q^2}{\Lambda^2}\right)^{-\tilde{\beta}_0/b} = \ln\left(\mathrm{e}\, u\, \mathrm{e}^{-\varepsilon(b)\, u}\right), \tag{4.27}$$

with $u = \varepsilon(b) + |b|^{-1}/\alpha^{(2)}(Q^2)$, and take:

$$Z(q) = -\varepsilon(b)\, \mathrm{e}^{-1}\, q^{-\tilde{\beta}_0/b} = -\varepsilon(b)\, \mathrm{e}^{-1-\frac{\tilde{\beta}_0}{b} \ln q}, \qquad q = Q^2/\Lambda^2, \tag{4.28}$$

then it follows from (4.27) that $Z = -\varepsilon(b)\, u\, \mathrm{e}^{-\varepsilon(b)\, u}$, giving with the help of (4.1):

$$W(Z(q)) = -\varepsilon(b)\, u = -1 - \frac{1}{b}\, \frac{1}{\widetilde{\alpha}^{(2)}(q)}, \qquad \widetilde{\alpha}^{(2)}(q) = \alpha^{(2)}(Q^2). \tag{4.29}$$

This yields the exact solution[3]:

$$\widetilde{\alpha}^{(2)}(q) = -\frac{1}{b}\,\frac{1}{[1+\mathcal{W}(q)]}\,, \qquad \mathcal{W}(q) = W(Z(q))\,. \tag{4.30}$$

In what follows, we shall denote $\alpha^{(2)}(Q^2)$ and $\widetilde{\alpha}^{(2)}(q)$ by $\alpha^{(2)}_{LW}(Q^2)$ and $\widetilde{\alpha}^{(2)}_{LW}(q)$ respectively. The requirement that $\alpha^{(2)}_{LW}(Q^2)$ is real and positive for a real positive Q^2 (at least for $Q^2 \gg \Lambda^2$) restricts $\mathcal{W}(q)$ to either the principal branch $W_0(Z(q))$ or $W_{-1}(Z(q))$, being the only branches that can take on real values. Now, depending on the sign of b, we can determine the relevant physical branch as follows:

1. if $b > 0$, i.e. $n_f \in [0,8]$, then for $q \geq 1$ we have $Z(q) \in [-1/\mathrm{e}, 0)$. In this interval, $W_{-1}(Z) \in (-\infty, -1]$ and $W_0(Z) \in [-1, 0)$. Hence, it is obvious that $W_{-1}(Z)$ is the physical branch. Note that in the UV limit $q \to \infty$, which corresponds to $Z \to 0^-$ and/or $W_{-1}(Z) \to -\infty$, we have $\widetilde{\alpha}^{(2)}_{LW} \to 0^+$ as required by asymptotic freedom. However, below the Landau singularity $q < 1$, the coupling $\alpha^{(2)}_{LW}$ is complex, indicating a break down in perturbation theory;

2. if $b < 0$, i.e. $n_f \in (8,16]$, then we have $Z(q) \in [0, \infty)$ for all $q \geq 0$. Hence, $W_0(Z)$ as being the only real and positive branch in this interval is the required physical branch. In the limit $q \to \infty$, $Z(q) \to \infty$ and accordingly $W_0(Z) \to \infty$, in which case we achieve the asymptotic freedom $\alpha^{(2)}_{LW} \to 0^+$. Here, at the IR limit $q \to 0$, which corresponds to $Z \to 0^+$ and/or $W_0(Z) \to 0^+$, we obtain an IR fixed point $\alpha^{(2)}_{LW}(0) = 1/|b|$ which is inaccessible by the 2-loop approximate expressions $\alpha^{(2)}_I(Q^2)$ and $\alpha^{(2)}_{\mathrm{PT}}(Q^2)$.

Now, we may rewrite the exact solution (4.30) as:

$$\widetilde{\alpha}^{(2)}_{LW}(q) = \begin{cases} -\dfrac{1}{b}\,\dfrac{1}{[1+W_{-1}(Z)]} & \text{for } n_f \in [0,8], \\ -\dfrac{1}{b}\,\dfrac{1}{[1+W_0(Z)]} & \text{for } n_f \in (8,16]. \end{cases} \tag{4.31}$$

This solution yields more accurate results than the standard approximate solutions $\alpha^{(2)}_I(Q^2)$ and $\alpha^{(2)}_{\mathrm{PT}}(Q^2)$. Furthermore, the latter can be obtained from (4.31) using the asymptotic

[3]For consistency with the notation used earlier in the analysis of the one-loop coupling, we shall use the same variable q to denote Q^2/Λ^2 throughout this chapter.

expression for the relevant branch of Lambert's W-function. So, for $b < 0$, we apply (4.21) at large positive $Z(q)$; while for $b > 0$, we use (4.15) at small negative $Z(q)$.

4.3 Singularity structure of the 2-loop coupling

Having explicitly derived the exact expression for the 2-loop coupling constant $\widetilde{\alpha}^{(2)}_{LW}(q)$, we shall now proceed to investigate its singularity structure in the complex $q-$plane. This requires the analytical continuation of $\widetilde{\alpha}^{(2)}_{LW}(q)$ to the whole complex q-plane, i.e. specifying the function $\mathcal{W}(q)$ in (4.30) for complex values of q. In what follows, our analysis would only cover the case $b > 0$ since it includes the phenomenologically interesting range of quark flavours $n_f \in [0, 8]$.

The main criterion we use for establishing the analytical continuation of the coupling $\widetilde{\alpha}^{(2)}_{LW}(q)$ to the complex $q-$plane is the requirement that the function $\widetilde{\alpha}^{(2)}_{LW}(q)$ remains single-valued and continuous, at least, throughout the region:

$$\mathcal{D} = \mathcal{D}^+ \cup \mathcal{D}^- = \{q : |q| > 1, -\pi < \arg(q) \leq \pi\}\,, \tag{4.32}$$

where

$$\mathcal{D}^+ = \{q : |q| > 1,\, 0 \leq \arg(q) \leq \pi\}, \qquad \mathcal{D}^- = \{q : |q| > 1,\, -\pi < \arg(q) < 0\}\,. \tag{4.33}$$

This requirement applies also to $\mathcal{W}(q)$ as it is explicitly related to $\widetilde{\alpha}^{(2)}_{LW}(q)$ by (4.30). For $q = |q|\,\mathrm{e}^{i\arg(q)}$ with the restriction $-\pi < \arg(q) \leq \pi$, equation (4.28) assumes the generic form:

$$Z(q) = \mathrm{e}^{-1-\upsilon \ln|q|}\ \mathrm{e}^{i\arg(Z(q))}\,, \tag{4.34}$$

where $\upsilon = \tilde{\beta}_0/b = \beta_0^2/\beta_1 \in [1.186, 48.167]$ for all $n_f \in [0, 8]$ and

$$\arg(Z) \in \{\vartheta_j^{\pm} : \vartheta_j^{\pm}(q) = \pm(2j-1)\,\pi - \upsilon \arg(q)\,,\ j \in \mathbb{Z}^+\}\,. \tag{4.35}$$

This clearly shows that there are some values of $\arg(q)$, υ and j for which $\arg(Z(q))$ is not

bounded by $\pm\pi$. On the other hand, however, we have by definition [4] that $\arg(Z)$ in the argument of $W_n(Z)$ is restricted to the interval $(-\pi, \pi]$. This indicates that we can not analytically continue the function $\mathcal{W}(q) = W(Z(q))$ to the whole complex $q-$plane, with the restriction that $\arg(Z(q)) \in (-\pi, \pi]$, unless it is described in a special way by more than one W_n-branch. Therefore, we think of $\mathcal{W}(q)$ as being made up of a finite number of W_n-branches, all subject to the following conditions:

1. each branch $W_n(Z(q))$ is described by a different $\arg(Z(q))$, i.e $\vartheta_j^{\pm}(q)$;

2. each branch $W_n(Z(q))$ is restricted to a distinct subinterval of $\arg(q)$ such that on this subinterval $\arg(Z(q))$ is bounded by $\pm\pi$;

3. each branch is chosen in such a way that keeps the whole set, i.e. $\mathcal{W}(q)$, continuous in $\mathcal{D}$ with the property that $\mathcal{W}(q) \to W_{-1}(Z(q))$ and $\arg(Z(q)) \to \pi$ as $\arg(q) \to 0$.

   N.B. the number of the relevant branches to be used in constructing $\mathcal{W}(q)$ is determined by the given value of v as we shall see later.

From the analyticity structure of Lambert's W-function, we can deduce the following relations between the adjacent W_n-branches across their boundaries, (where these boundaries all correspond to $\arg(Z) = \pm\pi$):

1. for the branch $n = -1$, we have at $\arg(Z) = \pi$

$$W_{-1}(|Z|\,\mathrm{e}^{i\,\pi}) = \begin{cases} W_1(|Z|\,\mathrm{e}^{-i\,\pi}) & \text{for } |Z| \leq 1/\mathrm{e} \\ W_0(|Z|\,\mathrm{e}^{-i\,\pi}) & \text{for } |Z| \geq 1/\mathrm{e}\ , \end{cases} \tag{4.36}$$

   while at $\arg(Z) = -\pi$, we have:

$$W_{-1}(|Z|\,\mathrm{e}^{-i\,\pi}) = W_{-2}(|Z|\,\mathrm{e}^{i\,\pi}); \tag{4.37}$$

2. for the branch $n = 1$, we have at $\arg(Z) = \pi$

$$W_1(|Z|\,\mathrm{e}^{i\,\pi}) = W_2(|Z|\,\mathrm{e}^{-i\,\pi})\,, \tag{4.38}$$

[4] By analogy with the nth branch of the complex logarithm $L_n(Z) = \ln|Z| + i\,(\arg(Z) + 2\pi\,n)$, which behaves exactly like $W_n(Z)$ for very large $|Z|$, $\arg(Z)$ in $W_n(Z)$ is restricted to the interval $(-\pi, \pi]$.

while at $\arg(Z) = -\pi$, we have:

$$W_1(|Z|\,e^{-i\,\pi}) = \begin{cases} W_{-1}(|Z|\,e^{i\,\pi}) & \text{for } |Z| \leq 1/e \\ W_0(|Z|\,e^{i\,\pi}) & \text{for } |Z| \geq 1/e\ ; \end{cases} \tag{4.39}$$

3. for any branch $n > 1$ or $n < -1$, we have at $\arg(Z) = \pm\pi$

$$W_n(|Z|\,e^{i\,\pi}) = W_{n+1}(|Z|\,e^{-i\,\pi}) \quad \text{and} \quad W_n(|Z|\,e^{-i\,\pi}) = W_{n-1}(|Z|\,e^{i\,\pi})\,; \tag{4.40}$$

4. for the principal branch $n = 0$, we have at $\arg(Z) = \pm\pi$ and $|Z| > 1/e$

$$W_0(|Z|\,e^{i\,\pi}) = W_1(|Z|\,e^{-i\,\pi}) \quad \text{and} \quad W_0(|Z|\,e^{-i\,\pi}) = W_{-1}(|Z|\,e^{i\,\pi})\,. \tag{4.41}$$

The above description of the behaviour of W_n across the cut helps in finding the right prescription for constructing, from the W_n-branches, the required function $\mathcal{W}(q)$ that complies with our proposed criterion for the analytical continuation of $\widetilde{\alpha}^{(2)}_{LW}(q)$ to the entire complex $q-$plane.

Now, we shall show how to determine the required function $\mathcal{W}(q)$, categorising our analysis according to the given value of υ as follows:

1. for $\upsilon < 2$, we take $\mathcal{W}(q) = W_{-1}(Z(q))$ with $\arg(Z) = \vartheta_1^+ = \pi - \upsilon\,\arg(q)$ in the upper half-plane $\mathrm{Im}\{q\} \geq 0$. This choice is made on the basis that when $\arg(q) = 0$ and $|q| > 1$, we obtain the relevant physical solution in (4.31). Also, having $\upsilon < 2$ in this case guarantees that $\vartheta_1^+ > -\pi$, i.e. ϑ_1^+ would never reach the cut of W_{-1} from below for all $\arg(q) \in [0, \pi]$. Therefore, $W_{-1}(Z(q))$ remains continuous for any $q \in \mathcal{D}^+$. In the lower half-plane $\mathrm{Im}\{q\} < 0$, on the other hand, we take $\mathcal{W}(q) = W_1(Z(q))$ with $\arg(Z) = \vartheta_1^- = -\pi - \upsilon\,\arg(q)$. In this way, we preserve the continuity of $\mathcal{W}(q)$ as we enter the region $\mathcal{D}^-$ from the upper edge of the positive q-axis. So, for $-\pi < \arg(q) \leq \pi$ the required function $\mathcal{W}(q)$ involves only two branches $W_{\pm 1}$ and assumes the form:

$$\mathcal{W}(q) = \begin{cases} W_1(Z_1^-(q)) & \text{for } -\pi < \arg(q) < 0 \\ W_{-1}(Z_1^+(q)) & \text{for } 0 \leq \arg(q) \leq \pi\,, \end{cases} \tag{4.42}$$

where

$$Z_l^-(q) = |Z(q)|\,\mathrm{e}^{i\,\vartheta_l^-(q)}\,, \qquad Z_l^+(q) = |Z(q)|\,\mathrm{e}^{i\,\vartheta_l^+(q)}\,, \quad l \in \mathbb{Z}^+\,. \tag{4.43}$$

2. for $\upsilon \geq 2$, we have a more complicated situation involving more than two W_n-branches in the determination of $\mathcal{W}(q)$. To simplify the argument, we begin by considering the easiest case $\upsilon \in [2,4)$. Now, it follows from (4.42) that each branch $W_{\pm 1}(Z_1^{\mp})$ would cross the cut in the $Z_1^{\mp}-$plane at $\arg(q) = \mp\frac{2\pi}{\upsilon}$, violating the requirement that $\arg(Z_1^{\mp}) \in (-\pi,\pi]$. To remedy this problem, we need to incorporate the two branches $W_{\pm 2}$ adjacent to $W_{\pm 1}$ in (4.42). Since $W_{\pm 1}(Z_1^{\mp}(q)) \to W_{\pm 2}(|Z|\mathrm{e}^{\mp i\,\pi})$ as $\arg(q) \to \mp\frac{2\pi}{\upsilon}$, which follows from (4.37) and (4.38), we let $\mathcal{W}(q) = W_2(Z_2^-(q))$ for $\arg(q) \in (-\pi, -\frac{2\pi}{\upsilon})$ and $\mathcal{W}(q) = W_{-2}(Z_2^+(q))$ for $\arg(q) \in [\frac{2\pi}{\upsilon}, \pi]$. In this way, we preserve the continuity of $\mathcal{W}(q)$ in $\mathcal{D}$. Now, we can write:

$$\mathcal{W}(q) = \begin{cases} W_2(Z_2^-(q)) & \text{for } -\pi < \arg(q) < -\frac{2\pi}{\upsilon} \\ W_1(Z_1^-(q)) & \text{for } -\frac{2\pi}{\upsilon} \leq \arg(q) < 0 \\ W_{-1}(Z_1^+(q)) & \text{for } 0 \leq \arg(q) < \frac{2\pi}{\upsilon} \\ W_{-2}(Z_2^+(q)) & \text{for } \frac{2\pi}{\upsilon} \leq \arg(q) \leq \pi\,. \end{cases} \tag{4.44}$$

In general, for $\upsilon \in \big[2N, 2N+2\big)$, where $N = 0, 1, 2, ..., 24$, we have:

$$\mathcal{W}(q) = \begin{cases} \mathcal{W}^-(q) & \text{for } -\pi < \arg(q) < 0 \\ \mathcal{W}^+(q) & \text{for } 0 \leq \arg(q) \leq \pi\,, \end{cases} \tag{4.45}$$

where

$$\mathcal{W}^{-}(q) = \begin{cases} W_{N+1}(Z^{-}_{N+1}(q)) & \text{for } -\pi < \arg(q) < -N\frac{2\pi}{\upsilon} \\ W_{N}(Z^{-}_{N}(q)) & \text{for } -N\frac{2\pi}{\upsilon} \le \arg(q) < -(N-1)\frac{2\pi}{\upsilon} \\ \vdots & \vdots \\ W_{n}(Z^{-}_{n}(q)) & \text{for } -n\frac{2\pi}{\upsilon} \le \arg(q) < -(n-1)\frac{2\pi}{\upsilon} \\ \vdots & \vdots \\ W_{2}(Z^{-}_{2}(q)) & \text{for } -\frac{4\pi}{\upsilon} \le \arg(q) < -\frac{2\pi}{\upsilon} \\ W_{1}(Z^{-}_{1}(q)) & \text{for } -\frac{2\pi}{\upsilon} \le \arg(q) < 0\,, \end{cases} \tag{4.46}$$

and

$$\mathcal{W}^{+}(q) = \begin{cases} W_{-1}(Z^{+}_{1}(q)) & \text{for } 0 \le \arg(q) < \frac{2\pi}{\upsilon} \\ W_{-2}(Z^{+}_{2}(q)) & \text{for } \frac{2\pi}{\upsilon} \le \arg(q) < \frac{4\pi}{\upsilon} \\ \vdots & \vdots \\ W_{-n}(Z^{+}_{n}(q)) & \text{for } (n-1)\frac{2\pi}{\upsilon} \le \arg(q) < n\frac{2\pi}{\upsilon} \\ \vdots & \vdots \\ W_{-N}(Z^{+}_{N}(q)) & \text{for } (N-1)\frac{2\pi}{\upsilon} \le \arg(q) < N\frac{2\pi}{\upsilon} \\ W_{-(N+1)}(Z^{+}_{N+1}(q)) & \text{for } N\frac{2\pi}{\upsilon} \le \arg(q) \le \pi\,. \end{cases} \tag{4.47}$$

Having constructed the required single-valued and continuous function $\mathcal{W}(q)$ in $\mathcal{D}$ from the W_n-branches, we shall now show that it has two branch cuts lying along the real intervals $\mathcal{B}_1 = \{q : 0 < \mathrm{Re}\, q \le 1, \mathrm{Im}\, q = 0\}$ and $\mathcal{B}_2 = \{q : \mathrm{Re}\, q \le 0, \mathrm{Im}\, q = 0\}$. To verify this, we begin by investigating the continuity of $\mathcal{W}(q)$ along the real $q-$axis. Depending on how we approach the positive real axis $\mathrm{Re}\, q > 0$, we find that:

$$\mathcal{W}(q) \to \begin{cases} W_1(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{-i\pi}) & \text{as } \arg(q) \to 0^- \\ W_{-1}(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{i\pi}) & \text{as } \arg(q) \to 0^+\,. \end{cases} \tag{4.48}$$

This allows us to obtain the following results:

1. for $|q| \geq 1$, we have from (4.36):

$$W_1(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{-i\pi}) = W_{-1}(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{i\pi})\,. \tag{4.49}$$

Hence, by substituting this into (4.48) we deduce the continuity of $\mathcal{W}(q)$, i.e. $\lim_{\arg(q)\to 0^+} \mathcal{W}(q) = \lim_{\arg(q)\to 0^-} \mathcal{W}(q)$.

2. for $|q| < 1$, we have from (4.36) and (4.39):

$$\begin{aligned} W_1(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{-i\pi}) &= W_0(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{i\pi})\,, \\ W_{-1}(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{i\pi}) &= W_0(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{-i\pi})\,. \end{aligned} \tag{4.50}$$

Using this in (4.48), we deduce the discontinuity of $\mathcal{W}(q)$ across $\mathcal{B}_1 \setminus \{1\}$ which can be represented as:

$$\lim_{\arg(q)\to 0^+} \mathcal{W}(q) - \lim_{\arg(q)\to 0^-} \mathcal{W}(q) = 2i\,\mathrm{Im}\Big\{W_0(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{i\pi})\Big\} \neq 0\,. \tag{4.51}$$

Here, we have simplified (4.51) by using the fact that:

$$\begin{aligned} \mathrm{Re}\Big\{W_0(x\,\mathrm{e}^{i\pi})\Big\} &= \mathrm{Re}\Big\{W_0(x\,\mathrm{e}^{-i\pi})\Big\}\,, \\ \mathrm{Im}\Big\{W_0(x\,\mathrm{e}^{i\pi})\Big\} &= -\mathrm{Im}\Big\{W_0(x\,\mathrm{e}^{-i\pi})\Big\}\,, \end{aligned} \tag{4.52}$$

for any $x > 1/\mathrm{e}$.

Due to (4.51), the interval $\mathcal{B}_1$ is excluded from the complex $q-$plane. As we move in a closed curve around $q = 1$ a discontinuity in $\mathcal{W}(q)$ would occur only if we crossed the cut $\mathcal{B}_1$, indicating that the point $q = 1$ is a branch point.

On the negative real axis $\mathrm{Re}\{q\} \leq 0$, i.e. $\mathcal{B}_2$, it is straightforward to see the discontinuity of $\mathcal{W}(q)$ from (4.45):

$$\begin{aligned} \lim_{\arg(q)\to\pi} \mathcal{W}(q) - \lim_{\arg(q)\to-\pi} \mathcal{W}(q) &= W_{-(N+1)}(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{i\pi(2N+1-\upsilon)}) \\ &\quad - W_{N+1}(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{-i\pi(2N+1-\upsilon)}) \\ &= 2i\,\mathrm{Im}\Big\{W_{-(N+1)}\,(\mathrm{e}^{-1-\upsilon \ln|q|}\,\mathrm{e}^{i\pi(2N+1-\upsilon)})\Big\} \neq 0\,. \end{aligned} \tag{4.53}$$

Here, we have used (4.13) to simplify (4.53).

At this stage, we conclude that the coupling constant $\widetilde{\alpha}^{(2)}_{LW}(q)$, as being defined by $\mathcal{W}(q)$ via (4.29), has the same analyticity structure in the complex $q-$plane as that of $\mathcal{W}(q)$, except at the branch point $q = 1$. Because, at this branch point $\mathcal{W} = -1$ in which case the denominator in (4.30) vanishes, resulting in the so-called Landau-pole singularity.

4.4 Non-perturbative analysis of the 2-loop coupling

The main purpose of this section is to remove the non-physical cut $\mathcal{B}_1$ together with the Landau-pole singularity from the exact 2-loop coupling $\widetilde{\alpha}^{(2)}_{LW}(q)$ without altering the correct UV properties. To achieve this goal, we apply our contour integral formula (2.41) to $\widetilde{\alpha}^{(2)}_{LW}(q)$ in the same way as we did in the one-loop case. Hence, by analogy with definition (2.43) we introduce our modified two-loop coupling as:

$$\bar{\alpha}^{(2)}(q,\lambda_e) = \frac{1}{\bar{\chi}^{(2)}(q,\lambda)}\bigg|_{\lambda=\lambda_e}, \tag{4.54}$$

where

$$\bar{\chi}^{(2)}(q,\lambda) = \frac{1}{2\pi i}\int_{C_{UV}} \frac{\mathrm{e}^{\lambda(k-q)}}{k-q}\,\frac{1}{\widetilde{\alpha}^{(2)}_{LW}(k)}\,dk\,. \tag{4.55}$$

For ease of calculation, we shall consider throughout the case in which the number of quark flavours $n_f \in [0,6]$, i.e. $\upsilon < 2$. A straightforward substitution of (4.30) for $\widetilde{\alpha}^{(2)}_{LW}(k)$ in (4.55) yields:

$$\bar{\chi}^{(2)}(q,\lambda) = -b - \frac{b}{2\pi i}\int_{C_{UV}} \frac{\mathrm{e}^{\lambda(k-q)}}{k-q}\,\mathcal{W}(k)\,dk\,. \tag{4.56}$$

Here $\mathcal{W}(k)$ is given by (4.42), which can be rewritten by using (4.13) as:

$$\mathcal{W}(k) = \begin{cases} W^{*}_{-1}(\mathrm{e}^{-1-\upsilon\ln|k|}\,\mathrm{e}^{i(\pi+\upsilon\arg k)}) & \text{for } -\pi < \arg k < 0 \\ W_{-1}(\mathrm{e}^{-1-\upsilon\ln|k|}\,\mathrm{e}^{i(\pi-\upsilon\arg k)}) & \text{for } 0 \le \arg k \le \pi\,. \end{cases} \tag{4.57}$$

Depending on the value of q, we shall now proceed to estimate the contour integral in (4.56). For $q > 1$, we use Cauchy's theorem to replace the UV-boundary C_{UV} with a small circle around q and a double keyhole shaped contour Γ surrounding the two cuts $\mathcal{B}_1$

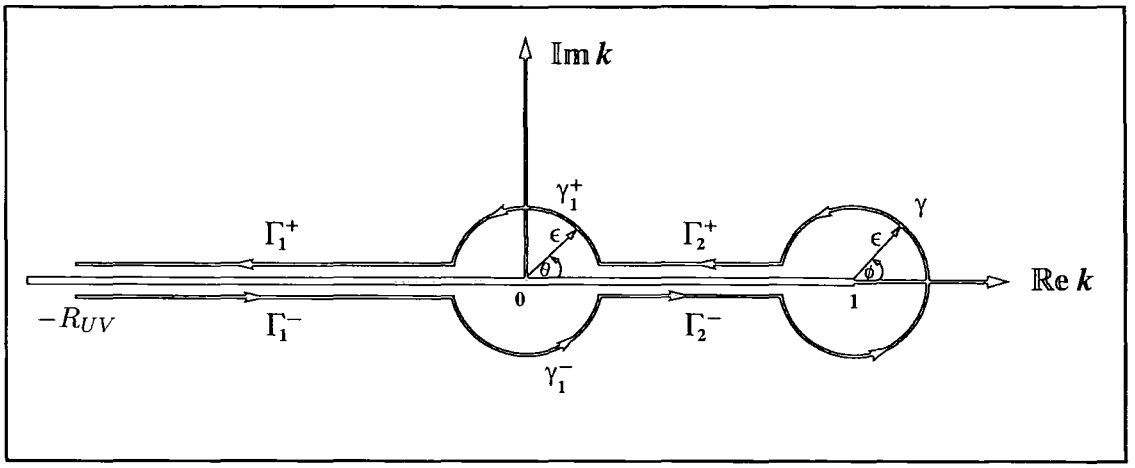


Figure 4.3: Sketch of the double keyhole shaped contour Γ. $\gamma_1^{\pm}$ and γ encircle the branch points at $k = 0$ and $k = 1$, respectively, and $\Gamma_1^{\pm}$ and $\Gamma_2^{\pm}$ surround the real intervals $(-R_{UV}, -\epsilon)$ and $(\epsilon, 1-\epsilon)$, respectively. The thick line represents the two connected branch cuts $\mathcal{B}_1 = (0, 1]$ and $\mathcal{B}_2 = (-\infty, 0]$.

and $\mathcal{B}_2$ as depicted in Fig.(4.3). In this way, we can write:

$$\bar{\chi}^{(2)}(q,\lambda) = -b - b\,\mathcal{W}(q) - b\,I_\Gamma(q,\lambda) = \frac{1}{\widetilde{\alpha}^{(2)}_{LW}(q)} - b\,I_\Gamma(q,\lambda)\,, \tag{4.58}$$

where

$$I_\Gamma(q,\lambda) = \frac{1}{2\pi i}\int_\Gamma \frac{e^{\lambda(k-q)}}{k-q}\,\mathcal{W}(k)\,dk\,. \tag{4.59}$$

Now, let us split Γ into seven components as depicted in Fig.(4.3), rewriting (4.59) as:

$$I_\Gamma(q,\lambda) = \frac{1}{2\pi i}\left[\int_{\Gamma_1^+ + \Gamma_1^-} + \int_{\Gamma_2^+ + \Gamma_2^-} + \int_{\gamma_1^+ + \gamma_1^-} + \int_{\gamma}\right]\frac{e^{\lambda(k-q)}}{k-q}\,\mathcal{W}(k)\,dk\,. \tag{4.60}$$

Here, as shown in appendix A, the contribution from integrating over the contours $\gamma_1^{\pm}$ and γ vanishes in the limit $\epsilon \to 0$. Thus, by taking the limits $\epsilon \to 0$ and $R_{UV} \to \infty$ we reduce (4.60) to two integrals on real intervals:

$$I_\Gamma(q,\lambda) = \int_0^\infty \frac{e^{-\lambda(k+q)}}{k+q}\,\mathcal{F}(k)\,dk + \int_0^1 \frac{e^{\lambda(k-q)}}{k-q}\,\mathcal{G}(k)\,dk\,, \tag{4.61}$$

where

$$\mathcal{F}(k) = \frac{1}{\pi}\,\mathrm{Im}\Big\{W_{-1}(e^{-1-v\ln k}\,e^{i\pi(1-v)})\Big\}\,, \tag{4.62}$$

and

$$\mathcal{G}(k) = \frac{1}{\pi}\,\mathrm{Im}\Big\{W_0(\mathrm{e}^{-1-\upsilon\ln k}\,\mathrm{e}^{i\pi})\Big\}\,. \tag{4.63}$$

The functions $2\pi i\mathcal{F}(k)$ and $2\pi i\mathcal{G}(k)$ represent the discontinuity of $\mathcal{W}(k)$ across the branch cuts $\mathcal{B}_1$ and $\mathcal{B}_2$, respectively. We remark that upon integrating along $\Gamma_2^{\pm}$ we have made use of the fact that for $k \in [0,1]$:

$$W_{-1}(\mathrm{e}^{-1-\upsilon\ln k}\,\mathrm{e}^{i\pi}) = W_0(\mathrm{e}^{-1-\upsilon\ln k}\,\mathrm{e}^{-i\pi}) = W_0^*(\mathrm{e}^{-1-\upsilon\ln k}\,\mathrm{e}^{i\pi})\,. \tag{4.64}$$

To determine the lower and upper bounds of $I_\Gamma(q,\lambda)$, we apply the mean-value theorem to both integrals in (4.61), obtaining:

$$I_\Gamma(q,\lambda) = \mathcal{F}(\hat{k}_1)\int_0^\infty \frac{\mathrm{e}^{-\lambda(k+q)}}{k+q}\,dk \;+\mathcal{G}(\hat{k}_2)\int_0^1 \frac{\mathrm{e}^{\lambda(k-q)}}{k-q}\,dk\,, \tag{4.65}$$

which after integration reduces to:

$$I_\Gamma(q,\lambda) = \mathcal{F}(\hat{k}_1)\,E_1(\lambda\,q) - \mathcal{G}(\hat{k}_2)\,[\,E_1(\lambda\,(q-1)) - E_1(\lambda\,q)\,]\,, \tag{4.66}$$

where $\hat{k}_1 \in [0,\infty)$ and $\hat{k}_2 \in [0,1]$. By using the fact that:

$$-(\upsilon+1) \le \mathcal{F}(\hat{k}_1) < -\upsilon \quad \text{and} \quad 0 \le \mathcal{G}(\hat{k}_2) \le 1\,, \tag{4.67}$$

we deduce from (4.66) the following result:

$$-E_1(\lambda\,(q-1)) - \upsilon\,E_1(\lambda\,q) \le I_\Gamma(q,\lambda) < -\upsilon\,E_1(\lambda\,q)\,. \tag{4.68}$$

This shows that for sufficiently large values of q the correction term $I_\Gamma(q,\lambda_e)$, at any given $\lambda = \lambda_e$, becomes negligible in comparison with the first term in (4.58), allowing $\bar{\alpha}^{(2)}(q,\lambda_e)$ in (4.54) to produce the correct UV behaviour.

Now, we shall return to (4.58) and consider the case when $q \in (0,1)$, i.e. q lying on the cut $\mathcal{B}_1$ as shown in Fig.(4.4). For these values of q, we replace the path of integration C_{UV}, using Cauchy's theorem, with the triple keyhole shaped contour $\widetilde{\Gamma}$ depicted in Fig.(4.4). In this way, we have:

$$\bar{\chi}^{(2)}(q,\lambda) = -b - b\,I_{\widetilde{\Gamma}}(q,\lambda)\,, \tag{4.69}$$

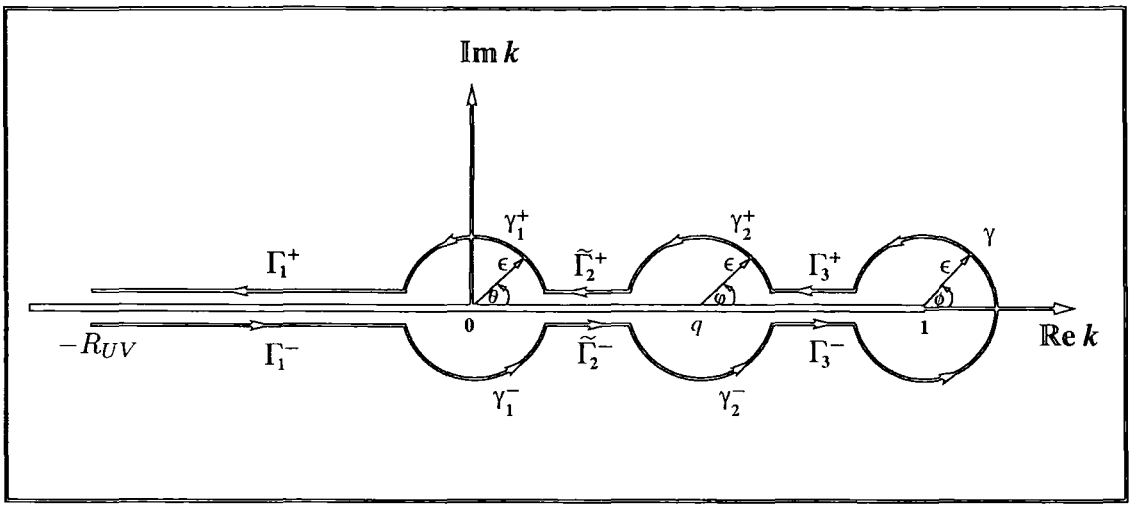


Figure 4.4: Sketch of the triple keyhole shaped contour $\widetilde{\Gamma}$. The thick line represents the two connected branch cuts $\mathcal{B}_1$ and $\mathcal{B}_2$.

where $I_{\widetilde{\Gamma}}(q,\lambda)$ is given by (4.59) with $\widetilde{\Gamma}$ being substituted for Γ. By analogy with (4.60), we write:

$$I_{\widetilde{\Gamma}}(q,\lambda) = \frac{1}{2\pi i}\left[\int_{\Gamma_1^+ + \Gamma_1^-} + \int_{\widetilde{\Gamma}_2^+ + \widetilde{\Gamma}_2^-} + \int_{\Gamma_3^+ + \Gamma_3^-} + \int_{\gamma_1^+ + \gamma_1^-} + \int_{\gamma_2^+ + \gamma_2^-} + \int_{\gamma}\right] \frac{e^{\lambda(k-q)}}{k-q}\, \mathcal{W}(k)\, dk\,, \tag{4.70}$$

where the contours $\Gamma_1^{\pm}$, $\widetilde{\Gamma}_2^{\pm}$, $\Gamma_3^{\pm}$, $\gamma_1^{\pm}$, $\gamma_2^{\pm}$ and γ are as illustrated in Fig.(4.4). In appendix A, we have shown that if $0 < q < 1$ the integrals along $\gamma_1^{\pm}$ and γ tend to zero as $\epsilon \to 0$. Also, we have calculated there the contribution from integrating over the semicircular arcs $\gamma_2^{\pm}$, giving:

$$\frac{1}{2\pi i}\lim_{\epsilon\to 0}\int_{\gamma_2^+ + \gamma_2^-} \frac{e^{\lambda(k-q)}}{k-q}\, \mathcal{W}(k)\, dk \;= \mathrm{Re}\,\{\mathcal{W}(q)\}\,, \qquad \text{for } q > 0\,. \tag{4.71}$$

Hence, in the limits $\epsilon \to 0$ and $R_{UV} \to \infty$, (4.70) reduces to:

$$I_{\widetilde{\Gamma}}(q,\lambda) = \mathrm{Re}\,\{\mathcal{W}(q)\} + \int_0^{\infty} \frac{e^{-\lambda(k+q)}}{k+q}\, \mathcal{F}(k)\, dk \;+ \int_0^{1} \frac{e^{\lambda(k-q)}}{k-q}\, \mathcal{G}(k)\, dk\,, \tag{4.72}$$

where the last term on the right hand side of (4.72) stands for the so-called Cauchy

principle value integral, defined as:

$$\fint_0^1 \frac{\mathrm{e}^{\lambda(k-q)}}{k-q}\,\mathcal{G}(k)\,dk = \lim_{\epsilon\to 0}\left[\int_0^{q-\epsilon}\frac{\mathrm{e}^{\lambda(k-q)}}{k-q}\,\mathcal{G}(k)\,dk + \int_{q+\epsilon}^1 \frac{\mathrm{e}^{\lambda(k-q)}}{k-q}\,\mathcal{G}(k)\,dk\right]. \tag{4.73}$$

Since $\mathcal{G}(k)$ is analytic at $k=q$, it is not difficult to show that the limit in (4.73) exists and has the value:

$$\begin{aligned}\fint_0^1 \frac{\mathrm{e}^{\lambda(k-q)}}{k-q}\,\mathcal{G}(k)\,dk &= -\mathcal{G}(q)\,\ln\left(\frac{q}{1-q}\right) + \int_0^1 \frac{\mathrm{e}^{\lambda(k-q)}\,\mathcal{G}(k)-\mathcal{G}(q)}{k-q}\,dk \\ &= -\mathcal{G}(q)\,\ln\left(\frac{q}{1-q}\right) + \int_0^1 \frac{\mathrm{e}^{\lambda(k-q)}-1}{k-q}\,\mathcal{G}(k)\,dk \\ &\quad + \int_0^1 \frac{\mathcal{G}(k)-\mathcal{G}(q)}{k-q}\,dk\,. \end{aligned}\tag{4.74}$$

Here, we note that the integrands of the first and second integrals in (4.74) tend to $\lambda\,\mathcal{G}(q)$ and $\mathcal{G}'(q)$, respectively, as $k\to q$, where $\mathcal{G}'(q)$, by use of (4.3), reads as:

$$\mathcal{G}'(q) = -\upsilon\,\frac{\mathcal{G}(q)}{q\,[\,[1+\mathrm{Re}\,W_0(\xi(q))]^2+\pi^2\,\mathcal{G}^2(q)\,]}\,, \qquad \xi(q) = -\mathrm{e}^{-1-\upsilon\ln q}\,. \tag{4.75}$$

This derivative exists for any $q\notin\{0,1\}$.

Now, we shall restrict our considerations to the two cases in which q coincides with the branch points of $\mathcal{W}$, i.e. $q=0$ and $q=1$. In both cases, (4.56) transforms under Cauchy's theorem to:

$$\bar{\chi}^{(2)}(q,\lambda) = -b - b\,I_\Gamma(q,\lambda)\,, \tag{4.76}$$

where $I_\Gamma(q,\lambda)$ is given by (4.60). For $q=1$, the integrals along $\gamma_1^{\pm}$ and γ in (4.60) tend to zero and $\mathcal{W}(1)=-1$, respectively, in the limit $\epsilon\to 0$, as shown in appendix A. This allows us to write:

$$\begin{aligned}\bar{\chi}^{(2)}(1,\lambda) &= -b\int_0^\infty \frac{\mathrm{e}^{-\lambda(k+1)}}{k+1}\,\mathcal{F}(k)\,dk \;-b\int_0^1 \frac{\mathrm{e}^{\lambda(k-1)}}{k-1}\,\mathcal{G}(k)\,dk\,, \\ &= -b\int_0^\infty \frac{\mathrm{e}^{-\lambda(k+1)}}{k+1}\,\mathcal{F}(k) - b\int_0^1 \frac{(\mathrm{e}^{\lambda(k-1)}-1)}{k-1}\,\mathcal{G}(k)\,dk - b\int_0^1 \frac{\mathcal{G}(k)}{k-1}\,dk\,. \end{aligned}\tag{4.77}$$

Here, the last integral over the finite interval [0,1] does exist although its integrand

$\mathcal{G}(k)/(k-1)$ is not bounded from above. To prove this, we use the variable transformation $k \to -\ln(1-k)$ to obtain:

$$\int_0^1 \frac{\mathcal{G}(k)}{k-1}\, dk = -\int_0^\infty \mathcal{G}(1-\mathrm{e}^{-k})\, dk\,, \tag{4.78}$$

where $\mathcal{G}(1-\mathrm{e}^{-k}) \to 0$ as $k \to \infty$. Now, observing that $\mathcal{G}(1-\mathrm{e}^{-k}) < 2/(1+k^2)$ for all $k \geq 0$, we deduce the following result:

$$\int_0^\infty \mathcal{G}(1-\mathrm{e}^{-k})\, dk < 2\int_0^\infty \frac{dk}{1+k^2} = \pi. \tag{4.79}$$

Hence, the integral in (4.78) converges to some number in the open interval $(-\pi, 0)$.

At this stage, recalling that $\mathrm{Re}\,\{\mathcal{W}(q)\} = \mathcal{W}(q) \leq -1$ for all $q \geq 1$, we conclude by inspection that (4.69), which we rewrite as:

$$\bar{\chi}^{(2)}(q,\lambda) = -b\left[1 + \mathrm{Re}\,\{\mathcal{W}(q)\} + \int_0^\infty \frac{\mathrm{e}^{-\lambda(k+q)}}{k+q}\mathcal{F}(k)\, dk + \int_0^1 \frac{\mathrm{e}^{\lambda(k-q)}}{k-q}\mathcal{G}(k)\, dk\right], \tag{4.80}$$

not only works for $q \in (0,1)$ but also applies to the case in which $q \geq 1$. We remark here that for $q > 1$ the Cauchy principal value symbol in (4.80) is no longer required because in this case we have no singularity on the finite interval of integration $[0,1]$.

Let us now return to (4.76) to calculate $\bar{\chi}^{(2)}(q,\lambda)$ for $q = 0$. To achieve this, we begin by computing (4.60) for $I_\Gamma(0,\lambda)$. Below, we express the various the contour integrals in (4.60), for $q = 0$, in terms of integrals along real intervals:

$$\frac{1}{2\pi i}\int_{\Gamma_1^+ + \Gamma_1^-} \frac{\mathrm{e}^{\lambda k}}{k}\mathcal{W}(k)\, dk = \int_1^{R_{UV}} \frac{\mathrm{e}^{-\lambda k}}{k}\mathcal{F}(k)\, dk + \int_\epsilon^1 \frac{(\mathrm{e}^{-\lambda k}-1)}{k}\mathcal{F}(k)\, dk + \int_\epsilon^1 \frac{\mathcal{F}(k)}{k}\, dk\,, \tag{4.81}$$

$$\frac{1}{2\pi i}\int_{\Gamma_2^+ + \Gamma_2^-} \frac{\mathrm{e}^{\lambda k}}{k}\mathcal{W}(k)\, dk = \int_\epsilon^{1-\epsilon} \frac{(\mathrm{e}^{\lambda k}-1)}{k}\mathcal{G}(k)\, dk + \int_\epsilon^{1-\epsilon} \frac{\mathcal{G}(k)}{k}\, dk\,, \tag{4.82}$$

$$\frac{1}{2\pi i}\int_{\gamma_1^+ + \gamma_1^-} \frac{e^{\lambda k}}{k} \mathcal{W}(k)\, dk = \frac{1}{\pi}\,\mathrm{Re}\left\{\int_0^\pi \left[e^{\lambda\epsilon\cos\theta}\, e^{i\lambda\epsilon\sin\theta} - 1\right] W_{-1}(e^{-1-v\ln\epsilon} e^{i(\pi - v\theta)})\, d\theta\right\}$$

$$+ \frac{1}{\pi}\,\mathrm{Re}\left\{\int_0^\pi W_{-1}(e^{-1-v\ln\epsilon}\, e^{i(\pi - v\theta)})\, d\theta\right\}. \qquad (4.83)$$

The integral along the circular contour γ in (4.60) is given by (A.16) in appendix A, where it is also shown to vanish as $\epsilon \to 0$ for all $q \neq 1$. Note that in (4.81), (4.82) and (4.83) we have subtracted out the singular part of each integral, appearing in the last term of each equation, to show later that their sum converges as $\epsilon \to 0$.

From (A.5) and the fact that $|e^{\lambda\epsilon\cos\theta}\, e^{i\lambda\epsilon\sin\theta} - 1| \leq e^{\lambda\epsilon} - 1$, we have:

$$\left|\int_0^\pi \left[e^{\lambda\epsilon\cos\theta}\, e^{i\lambda\epsilon\sin\theta} - 1\right] W_{-1}\,(e^{-1-v\ln\epsilon} e^{i(\pi - v\theta)})\, d\theta\right|$$

$$\leq \pi\,(e^{\lambda\epsilon} - 1)\left|W_{-1}(e^{-1-v\ln\epsilon} e^{i\pi(1-v)})\right|, \qquad (4.84)$$

which tends to zero as $\epsilon \to 0$. This shows that the first term in (4.83) would vanish in the limit $\epsilon \to 0$. Now, by summing (4.81), (4.82) and (4.83) and taking the limits $\epsilon \to 0$ and $R_{UV} \to \infty$, we obtain:

$$I_\Gamma(0,\lambda) = \int_1^\infty \frac{e^{-\lambda k}}{k}\,\mathcal{F}(k)\, dk + \int_0^1 \frac{(e^{-\lambda k} - 1)}{k}\,\mathcal{F}(k)\, dk + \int_0^1 \frac{(e^{\lambda k} - 1)}{k}\,\mathcal{G}(k)\, dk$$

$$+ \lim_{\epsilon\to 0}\left[\int_\epsilon^1 \frac{\mathcal{F}(k)}{k}\, dk + \int_\epsilon^{1-\epsilon} \frac{\mathcal{G}(k)}{k}\, dk + \frac{1}{\pi}\,\mathrm{Re}\left\{\int_0^\pi W_{-1}(e^{-1-v\ln\epsilon} e^{i(\pi - v\theta)})\, d\theta\right\}\right]. \qquad (4.85)$$

Here, the limit $\epsilon \to 0$ in (4.85) operates only after integrating and adding all the terms inside the two large brackets. To evaluate the last three integrals in (4.85), we make use of the following identities [5]:

$$\int \frac{W(e^{z_1 + z_2\ln x})}{x}\, dx = \frac{1}{z_2}\, W(e^{z_1 + z_2\ln x})\left[1 + \frac{1}{2}\, W(e^{z_1 + z_2\ln x})\right], \qquad (4.86)$$

$$\int W(r\, e^{i\theta})\, d\theta = -i\, W(r\, e^{i\theta})\left[1 + \frac{1}{2}\, W(r\, e^{i\theta})\right], \qquad (4.87)$$

[5] To evaluate the integrals in (4.86) and (4.87), we use the method of direct substitution, letting $u = W(e^{z_1 + z_2\ln x})$ and $v = W(r\, e^{i\theta})$ in (4.86) and (4.87) respectively. Then, from (4.3) it follows that $\frac{dx}{x} = \frac{1}{z_2}\,\frac{1+u}{u}\, du$ and $d\theta = -i\,\frac{1+v}{v}\, dv$. This gives $\int W(e^{z_1 + z_2\ln x})\,\frac{dx}{x} = \frac{1}{z_2} u(1 + u/2)$ and $\int W(r\, e^{i\theta})\, d\theta = -i\, v(1 + v/2)$.

together with the definitions (4.62) and (4.63). In this way, we obtain:

$$\begin{aligned}\int_\epsilon^1 \frac{\mathcal{F}(k)}{k}\,dk &= \frac{1}{\pi}\,\mathrm{Im}\int_\epsilon^1 W_{-1}(\mathrm{e}^{-1-\upsilon\ln k}\,\mathrm{e}^{i\pi(1-\upsilon)})\,\frac{dk}{k}\\ &= -\frac{1}{\upsilon}\,\mathcal{F}(1)\,[1+\pi\widetilde{\mathcal{F}}(1)] + \frac{1}{\upsilon}\,\mathcal{F}(\epsilon)\,[1+\pi\widetilde{\mathcal{F}}(\epsilon)],\end{aligned} \tag{4.88}$$

$$\begin{aligned}\int_\epsilon^{1-\epsilon} \frac{\mathcal{G}(k)}{k}\,dk &= \frac{1}{\pi}\,\mathrm{Im}\int_\epsilon^{1-\epsilon} W_0(\mathrm{e}^{-1-\upsilon\ln k}\,\mathrm{e}^{i\pi})\,\frac{dk}{k}\\ &= -\frac{1}{\upsilon}\,\mathcal{G}(1-\epsilon)\,[1+\pi\widetilde{\mathcal{G}}(1-\epsilon)] + \frac{1}{\upsilon}\,\mathcal{G}(\epsilon)\,[1+\pi\widetilde{\mathcal{G}}(\epsilon)],\end{aligned} \tag{4.89}$$

$$\frac{1}{\pi}\int_0^\pi \mathrm{Re}\left\{W_{-1}(\mathrm{e}^{-1-\upsilon\ln\epsilon}\,\mathrm{e}^{i(\pi-\upsilon\theta)})\right\}d\theta = -\frac{\mathcal{F}(\epsilon)}{\upsilon}\,[1+\pi\widetilde{\mathcal{F}}(\epsilon)] - \frac{\mathcal{G}(\epsilon)}{\upsilon}\,[1+\pi\widetilde{\mathcal{G}}(\epsilon)], \tag{4.90}$$

where

$$\widetilde{\mathcal{F}}(k) = \frac{1}{\pi}\,\mathrm{Re}\Big\{W_{-1}(\mathrm{e}^{-1-\upsilon\ln k}\,\mathrm{e}^{i\,\pi(1-\upsilon)})\Big\}, \tag{4.91}$$

and

$$\widetilde{\mathcal{G}}(k) = \frac{1}{\pi}\,\mathrm{Re}\Big\{W_0(\mathrm{e}^{-1-\upsilon\ln k}\,\mathrm{e}^{i\,\pi})\Big\}. \tag{4.92}$$

Now, combining (4.87), (4.88) and (4.89) and taking $\epsilon \to 0$ yields the value of the limit in (4.85), which is $-\frac{1}{\upsilon}\,\mathcal{F}(1)\,[1+\pi\widetilde{\mathcal{F}}(1)]$. At this stage, we substitute (4.85) into (4.76) to obtain:

$$\begin{aligned}\bar{\chi}^{(2)}(0,\lambda) = -b\Bigg[1 &- \frac{1}{\upsilon}\,\mathcal{F}(1)\,[1+\pi\widetilde{\mathcal{F}}(1)] + \int_1^\infty \frac{\mathrm{e}^{-\lambda k}}{k}\,\mathcal{F}(k)\,dk\\ &+ \int_0^1 \frac{(\mathrm{e}^{-\lambda k}-1)}{k}\,\mathcal{F}(k)\,dk + \int_0^1 \frac{(\mathrm{e}^{\lambda k}-1)}{k}\,\mathcal{G}(k)\,dk\Bigg].\end{aligned} \tag{4.93}$$

Using Gauss-Legendre and Gauss-Laguerre quadrature rules for computing definite and semi-infinite integrals, respectively, we evaluate $\bar{\chi}^{(2)}(0,\lambda)$ numerically for any given $\lambda > 0$. In Fig.(4.5), we plot the functional variation of $\bar{\chi}^{(2)}(0,\lambda)$ with λ for $n_f = 3$. The figure shows that function $\bar{\chi}^{(2)}(0,\lambda)$ is monotonically decreasing and changes sign as λ crosses some point near 0.88. The $\lambda-$dependence of $\bar{\chi}^{(2)}(0,\lambda)$ remains almost the same for all $n_f \in [0,6]$. In table (4.1), we list the zeros of $\bar{\chi}^{(2)}(0,\lambda)$, denoted by $\widehat{\lambda}$, for different values of n_f. Now, from the positivity of $\bar{\alpha}^{(2)}(0,\lambda)$ we expect the effective parameter λ_e

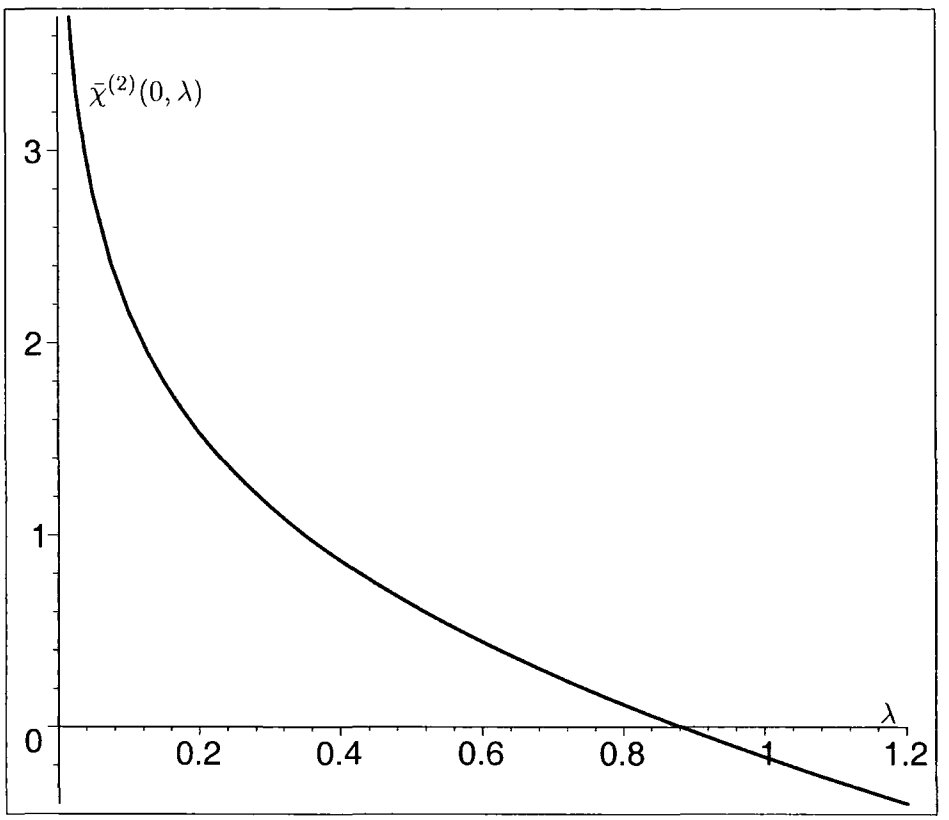


Figure 4.5: The variation of $\bar{\chi}^{(2)}(0,\lambda)$ versus λ for $n_f = 3$.

n_f	0	1	2	3	4	5	6
$\widehat{\lambda}$	0.8896	0.8888	0.8866	0.8824	0.8750	0.8621	0.8382

Table 4.1: The zeros of $\bar{\chi}^{(2)}(0,\lambda)$, up to 4-decimal places, for different n_f.

to lie somewhere in the open interval $(0,\widehat{\lambda})$. For simplicity, we take $\lambda_e \in (0, 0.8]$ for all n_f under consideration. This interval is only slightly wider than its counterpart in the one-loop case.

4.5 A ballpark estimate of the 2-loop λ_e

In this section we give a rough estimate of the value of the effective parameter λ_e, following similar guidelines to those used in the one-loop case.

For ease of calculation, we shall try to extract λ_e from the behaviour of $\bar{\chi}^{(2)}(q,\lambda)$ rather than $\bar{\alpha}^{(2)}(q,\lambda)$. Starting from (4.58) and (4.68), we deduce that the function $\bar{\chi}^{(2)}(q,\lambda)$ tends to $\chi^{(2)}_{LW}(q) = 1/\widetilde{\alpha}^{(2)}_{LW}(q)$ very rapidly, for any given $q > 1$, as λ increases toward

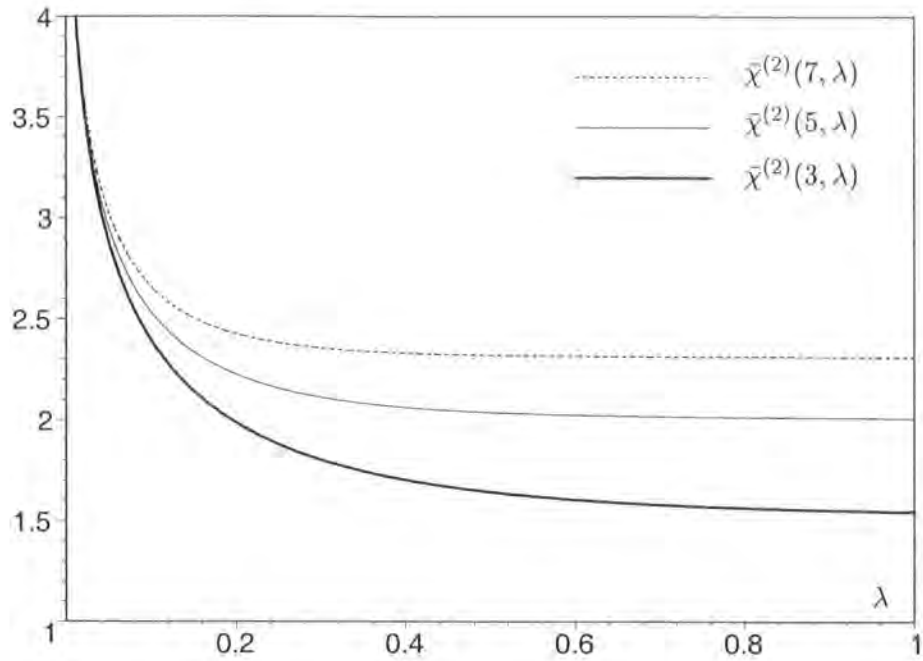


Figure 4.6: The variation of $\bar{\chi}^{(2)}(q,\lambda)$ versus λ for $q = 3$, 5 and 7 with $n_f = 3$.

infinity. This is illustrated in Fig.(4.6) for $q = 3$, 5 and 7 with $n_f = 3$. The way in which $\bar{\chi}^{(2)}(q,\lambda)$ varies with λ, for any given $q > 1$ and $n_f \in [0,6]$, gives an illustrative example of case(3) qualitatively demonstrated by the graph in Fig.(2.5). Given $\alpha^{(2)}_{\rm PT}(Q^2) > \alpha^{(3)}_{\rm PT}(Q^2)$, see Fig.(2.8) in chapter 2 and the discussion therein, we expect the perturbative estimate $\chi^{(2)}_{LW}(q)$ to undershoot the reciprocal of the true value of the coupling constant $\alpha(q)$, at least for small and moderate values of q. This indicates that our problem is of the type classified in chapter 2 by case(3.b), which is depicted in Fig.(2.5/3.b). Hence, by analogy with this case, we may claim that for every point $q > 1$ for which $\chi^{(2)}_{LW}(q)$ requires reasonable corrections there exists a proper value $\lambda = \lambda_0(q)$ such that $\bar{\chi}^{(2)}(q,\lambda_0(q)) = 1/\alpha(q)$. In an approximation similar to that used in the one-loop case, we think of $\lambda_0(q)$ as the value at which the curvature function $K^{(2)}(\lambda,q)$ of $\bar{\chi}^{(2)}(q,\lambda)$, for a given $q > 1$, is a local maximum. Here, $K^{(2)}(\lambda,q)$ is given by:

$$K^{(2)}(\lambda,q) = \frac{|\bar{\chi}^{(2)}_{\lambda\lambda}(q,\lambda)|}{\Big[\,1 + (\bar{\chi}^{(2)}_{\lambda}(q,\lambda))^2\,\Big]^{3/2}}, \tag{4.94}$$

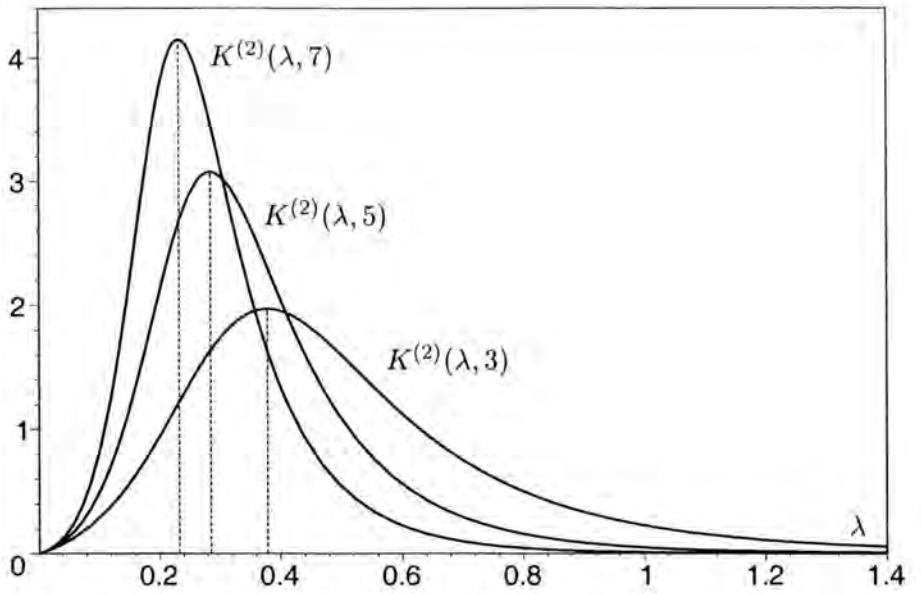


Figure 4.7: The variation of $K^{(2)}(\lambda, q)$ versus λ for $q = 3$, 5 and 7, using $n_f = 3$.

where $\bar{\chi}^{(2)}_{\lambda} = \partial\bar{\chi}^{(2)}/\partial\lambda$ and $\bar{\chi}^{(2)}_{\lambda\lambda} = \partial^2\chi^{(2)}/\partial\lambda^2$ are given as:

$$\bar{\chi}^{(2)}_{\lambda}(q,\lambda) = -b\,\mathrm{e}^{-\lambda q}\left[\int_0^1 \mathrm{e}^{\lambda k}\,\mathcal{G}(k)\,dk - \int_0^\infty \mathrm{e}^{-\lambda k}\,\mathcal{F}(k)\,dk\right], \tag{4.95}$$

$$\bar{\chi}^{(2)}_{\lambda\lambda}(q,\lambda) = -b\,\mathrm{e}^{-\lambda q}\left[\int_0^1 \mathrm{e}^{\lambda k}\,\mathcal{G}(k)\,(k-q)\,dk + \int_0^\infty \mathrm{e}^{-\lambda k}\,\mathcal{F}(k)\,(k+q)\,dk\right]. \tag{4.96}$$

In Fig.(4.7), using $n_f = 3$, we plot the curvature function $K^{(2)}(\lambda, q)$ against λ for $q = 3$, 5 and 7, showing the value $\lambda_0(q)$ at which $K^{(2)}(\lambda, q)$ is a local maximum by a vertical dashed line. Using $\lambda_0(q)$ in $\bar{\chi}^{(2)}(q,\lambda)$ in regions where perturbation theory is not trustworthy gives a better approximation than $\chi^{(2)}_{LW}(q)$ because there we would expect the estimate of $\chi^{(2)}_{LW}(q)$ to significantly undershoot the true value $1/\alpha(q)$. This is illustrated in Fig.(4.8) with $\bar{\chi}^{(2)}(3,\lambda)$ for $n_f = 3$, using $\lambda_0(3) = 0.379$.

By plotting the function $\lambda_0(q)$ on the interval $q > 1$ for any $n_f \in [0, 6]$, we find that it is a monotonically decreasing function of q, just as illustrated in Fig.(4.9). We also observe that the magnitude of $\lambda_0(q)$ calculated for any $q > 1$ lies within the previously specified λ-interval of positivity of $\bar{\chi}^{(2)}(q,\lambda)$ when $q < 1$. The distinction between $\bar{\chi}^{(2)}(q, \lambda_0(q))$ and $\chi^{(2)}_{LW}(q)$ decreases with increasing q, indicating the absence of any significant improvement

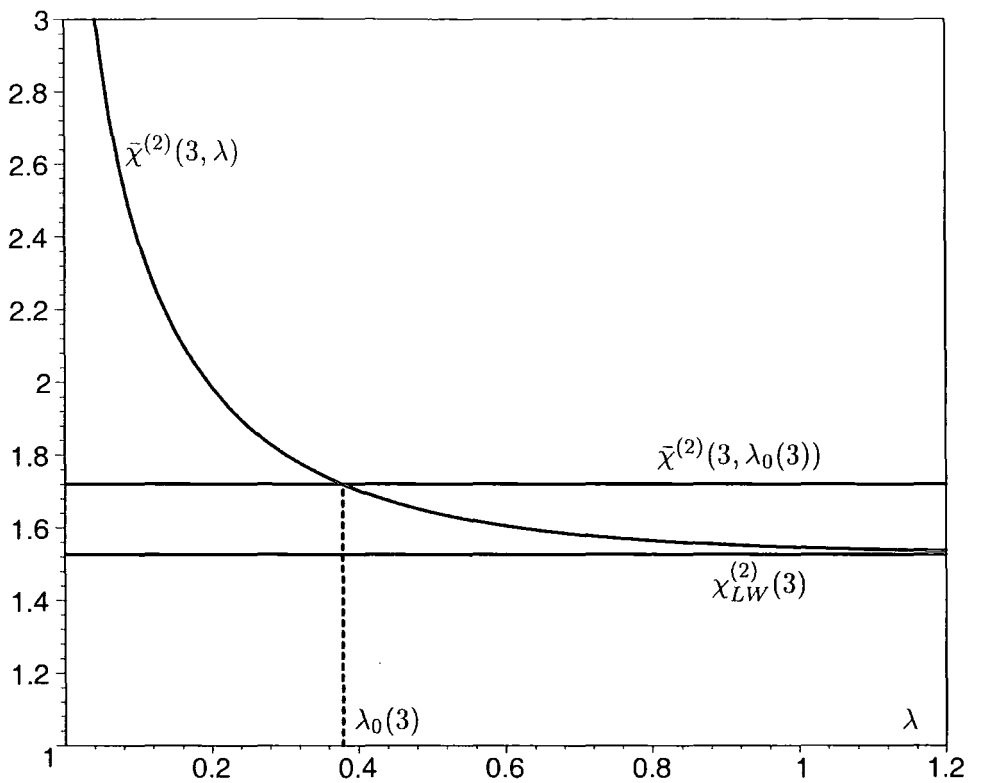


Figure 4.8: The variation of $\bar{\chi}^{(2)}(3,\lambda)$ versus λ for $n_f = 3$.

on the perturbative estimate $\chi^{(2)}_{LW}(q)$ at sufficiently large values of q. Practically, for $q \geq 150$ and $n_f \in [0,6]$ we find that $\bar{\chi}^{(2)}(q,\lambda_0(q)) \cong \chi^{(2)}_{LW}(q)$ within two decimal places of accuracy, which is inside the bounds of physical interest. Hence, we shall only consider those values of $\lambda_0(q)$ corresponding to the $q-$domain $\{q : 1 < q < 150\}$ over which the difference between $\bar{\chi}^{(2)}(q,\lambda_0(q))$ and $\chi^{(2)}_{LW}(q)$ is appreciable. On this basis, we shall seek to find λ_e in an interval $(\lambda_0(150),\lambda_0(1))$ which is narrower than the previously suggested one. For $n_f = 3$, we would expect $\lambda_e \in (\lambda_0(150),\lambda_0(1)) = (0.0253, 0.5838) \subset (0, 0.8]$.

As illustrated in Fig.(4.9), $\lambda_0(q)$ is a slowly varying function in a large subinterval $(25, 150)$ of the region where we suspect to find λ_e. Therefore, by analogy with the one-loop case, we take the average of $\lambda_0(q)$ over the selected interval $1 < q < 150$ to represent our closest estimate to λ_e. Having done that, using $n_f = 3$, we obtain $\lambda_e = 0.07$. Repeating the same analysis with different n_f does not result in any value for λ_e that differ significantly from 0.07. Therefore, we shall use this value as an approximation to λ_e for all $n_f \in [0,6]$.

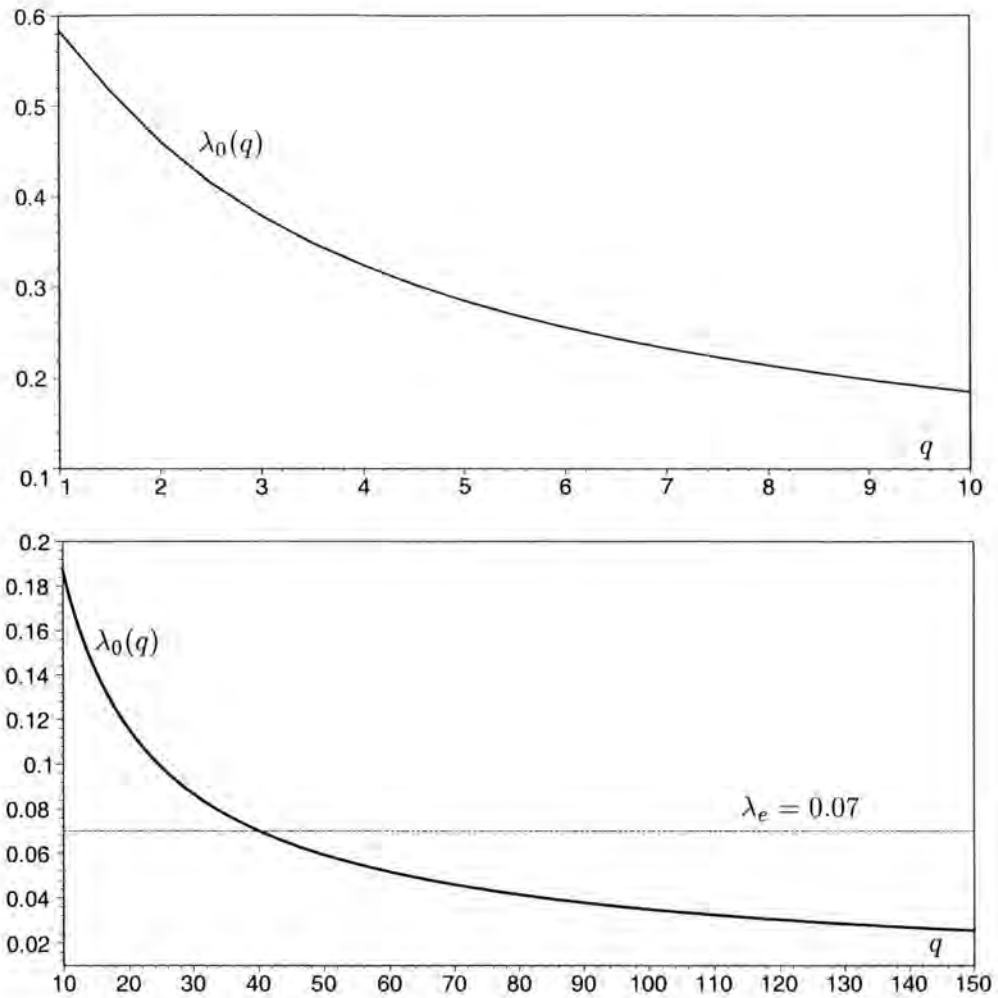


Figure 4.9: The variation of $\lambda_0(q)$ versus q for $n_f = 3$.

4.6 Results and discussion

In this section, we shall display our results through a comparison with the predictions of the standard perturbation theory and the new background field formalism explained in Ref. [15]. We shall also compare our 2-loop formula for the running coupling constant $\bar{\alpha}^{(2)}(q, \lambda_e) = 1/\bar{\chi}^{(2)}(q, \lambda_e)$ with the behaviour of the exact 2-loop Lambert's W-solution $\widetilde{\alpha}^{(2)}_{LW}(q)$ in the q-plane.

From now on, we shall denote $\bar{\alpha}^{(2)}(q,\lambda_e)$ for $\lambda_e = 0.07$ by $\bar{\alpha}^{(2)}(q)$ and write:

$$\bar{\alpha}^{(2)}(q) = -\frac{1}{b}\,\frac{1}{\left[1 + \mathrm{Re}\,\{\mathcal{W}(q)\} + \bar{\Upsilon}_{\mathrm{IR}}(q)\right]}\,, \tag{4.97}$$

where $\mathcal{W}(q)$ is given by (4.57) which for real and positive q reduces to:

$$\mathcal{W}(q) = W_{-1}(-\mathrm{e}^{-1-\upsilon \ln q})\,, \tag{4.98}$$

and

$$\bar{\Upsilon}_{\mathrm{IR}}(q) = \int_0^\infty \frac{\mathrm{e}^{-\lambda_e(k+q)}}{k+q}\,\mathcal{F}(k)\,dk + \int_0^1 \frac{\mathrm{e}^{\lambda_e(k-q)}}{k-q}\,\mathcal{G}(k)\,dk. \tag{4.99}$$

Here, $\bar{\Upsilon}_{\mathrm{IR}}(q)$ represents the IR contribution to the exact 2-loop expression $\widetilde{\alpha}^{(2)}_{LW}(q)$. Note that for $q > 1$, $\bar{\Upsilon}_{\mathrm{IR}}(q)$ reduces to (4.61) and as a result it follows from (4.68) that:

$$-E_1(\lambda_e\,(q-1)) - \upsilon\,E_1(\lambda_e\,q) \leq \bar{\Upsilon}_{\mathrm{IR}}(q) < -\upsilon\,E_1(\lambda_e\,q)\,, \quad \text{for} \quad q > 1\,. \tag{4.100}$$

Here, $\upsilon = \beta_0^2/\beta_1 \in [1.186, 1.885]$ for $n_f \in [0,6]$. Since $E_1(x)$ is a rapidly monotonic decreasing function in x, we deduce from (4.100) that for sufficiently large values of q the contribution of $\bar{\Upsilon}_{\mathrm{IR}}(q)$ becomes negligible in comparison with the additive term $(1 + \mathrm{Re}\,\{\mathcal{W}(q)\})$ in the denominator of (4.97), in which case $\bar{\alpha}^{(2)}(q)$ tends to $\widetilde{\alpha}^{(2)}_{LW}(q)$ producing the correct UV behaviour.

In Fig.(4.10), we give an illustrative comparison between our formula $\bar{\alpha}^{(2)}(q)$ and its perturbative counterpart $\widetilde{\alpha}^{(2)}_{LW}(q)$ using $n_f = 3$ as the average number of active quarks. This figure shows how the 3−flavour coupling constant in our approach differs dramatically from the 2-loop perturbative expression $\widetilde{\alpha}^{(2)}_{LW}(q)$ as q enters the IR region, $0 \leq q \leq 1$, or its extended neighbourhood, illustrating the absence of the ghost pole problem and the presence of the property of asymptotic freedom in our model. In Fig.(4.11), we demonstrate the explicit energy dependence of the coupling constant in our approach $\bar{\alpha}^{(2)}_{LW}(Q^2) = \bar{\alpha}^{(2)}(Q^2/\Lambda^2)$, giving a direct comparison with the 2- and 3-loop coupling constants $\alpha^{(2)}_{\mathrm{PT}}(Q^2)$ and $\alpha^{(3)}_{\mathrm{PT}}(Q^2)$ of the standard perturbation theory and the 2-loop coupling $\alpha^{(2)}_{B}(Q^2)$ derived from the new background field formalism [15]. For our expression $\bar{\alpha}^{(2)}_{LW}(Q^2)$ we employ $\Lambda^{(3)} = 0.502$ GeV and $\Lambda^{(4)} = 0.402$ GeV below and above the energy threshold $Q_{th} = 2m_c = 2.70$ GeV, respectively. These values are calculated from

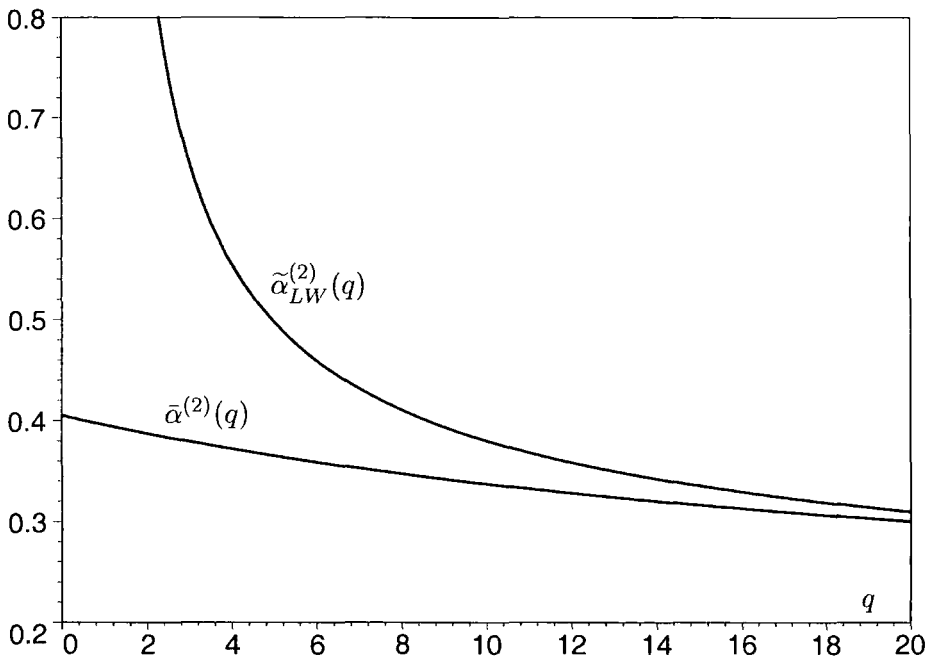


Figure 4.10: The $q-$behaviour of our model $\bar{\alpha}^{(2)}(q)$ for the coupling constant plotted against its perturbative counterpart $\widetilde{\alpha}^{(2)}_{LW}(q)$, using $n_f = 3$.

the matching condition introduced by (3.2) using $\Lambda^{(5)}_{\rm PT} = 0.274$ GeV as the starting value of the matching procedure, as explained in chapter 3. As for the perturbative expressions plotted in Fig.(4.11.a), i.e. $\alpha^{(2)}_{\rm PT}(Q^2)$ and $\alpha^{(3)}_{\rm PT}(Q^2)$, we use the values of $\Lambda^{(n_f)}_{\rm PT}$ summarised in Table(4.2). In this table, the values of $\Lambda^{(3)}_{\rm PT}$ in the first column are derived in

n_f	3	4
$\Lambda^{(n_f)}_{\rm PT}$ GeV 2-loop order	0.495	0.4057
$\Lambda^{(n_f)}_{\rm PT}$ GeV 3-loop order	0.383	0.3134

Table 4.2: The values of $\Lambda^{(n_f)}_{\rm PT}$ in the 2- and 3-loop order perturbation theory

chapter 2 from (2.68) whereas the values of $\Lambda^{(4)}_{\rm PT}$ in the second column are calculated from the matching procedure, using the values of $\Lambda^{(3)}_{\rm PT}$.

In Fig.(4.11), we observe that our formula $\bar{\alpha}^{(2)}_{LW}(Q^2)$ incorporates both the IR freezing property and the correct UV behaviour. Below 200 MeV our coupling $\bar{\alpha}^{(2)}_{LW}(Q^2)$ freezes rapidly to a constant value of 0.405, which differs by 42.55 % from the value of $\alpha^{(2)}_B(0) =$

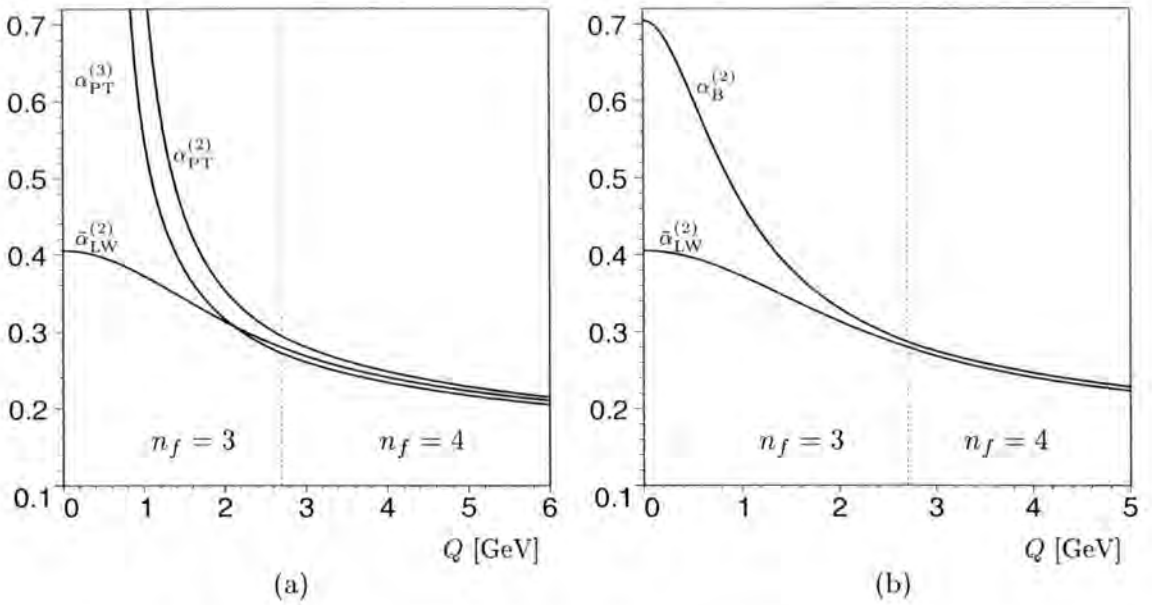


Figure 4.11: the energy dependence of the coupling constant in our approach $\bar{\alpha}^{(2)}_{LW}(Q^2)$ compared to those in (a) perturbation theory, i.e. $\alpha^{(2)}_{\rm PT}(Q^2)$ and $\alpha^{(3)}_{\rm PT}(Q^2)$, and (b) the background field formalism $\alpha^{(2)}_{B}(Q^2)$. The dashed vertical lines are to indicate the energy threshold at $2m_c = 2.70$ GeV.

n_f	0	1	2	3	4	5
$\bar{\alpha}^{(2)}_{\rm LW}(0)$	0.326	0.348	0.374	0.405	0.445	0.497
$\alpha^{(2)}_{B}(0)$	0.713	0.713	0.714	0.705	0.576	0.447

Table 4.3: The values of $\bar{\alpha}^{(2)}_{\rm LW}(0)$ compared to those of $\alpha^{(2)}_{B}(0)$

0.705 as shown in Fig.(4.11.b). In our approach, the value of $\bar{\alpha}^{(2)}_{LW}(Q^2)$ at the low energy scale $Q = 1.0 \pm 0.2$ GeV is found to be $\bar{\alpha}^{(2)}_{LW}(Q^2) = 0.396 \mp 0.002$. This is in good agreement with the result $\alpha_s(Q^2) = 0.38 \pm 0.03(exp) \pm 0.04(theory)$ extracted from the fits to charmonium spectrum and fine structure splittings at the same energy scale [37].

In Table(4.3), we list the values of the IR fixed-points in our approach and the background field formalism for $n_f = [0, 5]$. Here, we remark that for all n_f the values of $\bar{\alpha}^{(2)}_{LW}(0)$ are independent of the mass scale parameter Λ.

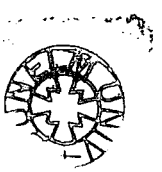
Chapter 5

The Schrödinger Vacuum and Analyticity Structure

5.1 Introduction

Although the field theoretic Schrödinger representation [52–55] is a natural context for developing non-perturbative methods in quantum field theory, and provides useful analogs of the conventional techniques and concepts in quantum mechanics, it has not received the same attention as the canonical quantisation approach. This is partly due to the popularity of the latter in which space-time symmetries are displayed manifestly, and partly because the existence of vacuum wave-functionals in the Schrödinger representation with diagonal field operators was only shown by Symanzik as late as 1981 [56]. Nonetheless, there has been growing interest in the subject as a result of the search for new tools in field theory and also because the Schrödinger representation is implicit in much recent work on field theories defined on space-times with boundaries, see for example [58]. Moreover, This representation provides a framework for novel approaches to the solution of quantum field theories, for example in the use of variational principles [59] to model states and describe non-perturbative phenomena.

We begin this chapter by giving a detailed study of the Schrödinger representation in quantum field theory, showing how the vacuum wave-functionals are developed. We shall illustrate explicitly how to calculate the unrenormalised vacuum functional for the ϕ^4-theory to one-loop order. Then, we present our objectives, introducing a further appli-



cation of our approach in the area of wave functionals. We show that for an interacting scalar field theory with a non-zero mass gap the Schrödinger vacuum functional $\Psi_0[\varphi]$ undergoes a significant simplification when evaluated for fields $\varphi(x)$ whose Fourier transforms $\widetilde{\varphi}(k)$ have sufficiently small supports. As we will show this is because its logarithm $\mathsf{W}_0[\varphi]$ reduces to a local functional expansion, i.e. a single spatial integral of a sum of terms each composed of $\varphi(x)$ and/or a finite number of its derivatives at the same spatial point. A knowledge of this expansion or its leading terms enables us to estimate the vacuum $\Psi_0[\varphi] = \exp\big(\mathsf{W}_0[\varphi]\big)$ for an arbitrary source field by exploiting the analyticity of $\mathsf{W}_0[\varphi_s]$ in a complex scale parameter s, where $\varphi_s = \varphi(x/\sqrt{s})$. By studying the analyticity of W_0 for the scaled field φ_s, we find that it extends to an analytic function of s on the whole of the complex s-plane with a branch cut restricted to the negative real axis. This property of analyticity in the complex s-plane is the basis of our method because it allows the use of Cauchy's theorem for relating the large-s behaviour, where the local expansion of $\mathsf{W}_0[\varphi_s]$ holds, to the point $s = 1$.

5.2 Field Theoretic Schrödinger Representation

In this section, we shall review the Schrödinger formulation of quantum field theory in Minkowski space-time, showing that it is a natural extension of non-relativistic quantum mechanics familiar from atomic physics. For the sake of simplicity, however, we shall consider only neutral massive scalar fields.

The Lagrangian density for a free and spinless scalar field $\phi(x)$ with mass m, in 4-dimensional Minkowski space-time $x = (\mathbf{x}, t)$, reads as [52]:

$$\mathcal{L}_0 = \frac{1}{2}\,\partial_\mu\phi(x)\partial^\mu\phi(x) - \frac{1}{2}\,m^2\,\phi^2(x) = \frac{1}{2}\,\Big(\,\dot{\phi}^2 - (\nabla\phi)^2 - m^2\,\phi^2\,\Big)\,, \tag{5.1}$$

where the dot on ϕ denotes differentiation with respect to time. The canonical momentum conjugate to the field $\phi(x)$ is defined by:

$$\pi(x) = \frac{\partial\mathcal{L}_0}{\partial\dot{\phi}} = \dot{\phi}(x)\,, \tag{5.2}$$

and the Hamiltonian density $\mathcal{H}_0$ is constructed as:

$$\mathcal{H}_0 = \pi(x)\,\dot{\phi}(x) - \mathcal{L}_0\,. \tag{5.3}$$

This allows us to write the associated Hamiltonian H_0 as a functional of ϕ and π:

$$\begin{aligned} H_0[\phi,\pi;t] &= \frac{1}{2}\int d^3\mathbf{x}\ \left[\,\pi^2(\mathbf{x},t) + (\nabla\phi(\mathbf{x},t))^2 + m^2\,\phi^2(\mathbf{x},t)\,\right] \\ &= \frac{1}{2}\int d^3\mathbf{x}\ \left[\,\pi^2(\mathbf{x},t) + \phi(\mathbf{x},t)\,(-\nabla^2 + m^2)\,\phi(\mathbf{x},t)\,\right]\,, \end{aligned} \tag{5.4}$$

which depends on time only through the field and its momentum conjugate. Here, the field $\phi(\mathbf{x},t)$ is assumed to vanish on the surface boundary of Minkowski space.

The Euler-Lagrange equations of motion for this system lead to the well-known Klein-Gordon equation:

$$(\partial_\mu\partial^\mu + m^2)\phi(x) = 0\,, \tag{5.5}$$

which has the classical solution:

$$\phi(\mathbf{x},t) = \int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{1}{\sqrt{2\omega_\mathbf{p}}}\left[a(\mathbf{p})\,\mathrm{e}^{i(\mathbf{p}.\mathbf{x}-\omega_\mathbf{p}t)} + a^*(\mathbf{p})\,\mathrm{e}^{-i(\mathbf{p}.\mathbf{x}-\omega_\mathbf{p}t)}\right]\,, \tag{5.6}$$

where

$$\omega_\mathbf{p} \equiv \omega(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m^2}\,. \tag{5.7}$$

Since $\pi(\mathbf{x},t) = \dot{\phi}(\mathbf{x},t)$, differentiating (5.6) with respect to time gives:

$$\pi(\mathbf{x},t) = -i\int \frac{d^3\mathbf{p}}{(2\pi)^3}\sqrt{\frac{\omega_\mathbf{p}}{2}}\left[a(\mathbf{p})\,\mathrm{e}^{i(\mathbf{p}.\mathbf{x}-\omega_\mathbf{p}t)} - a^*(\mathbf{p})\,\mathrm{e}^{-i(\mathbf{p}.\mathbf{x}-\omega_\mathbf{p}t)}\right]\,. \tag{5.8}$$

Now, the system can be canonically quantised by treating the classical fields ϕ and π as operators, satisfying the equal-time commutation relations:

$$[\hat{\phi}(\mathbf{x},t),\hat{\pi}(\mathbf{x}',t)] = i\delta(\mathbf{x}-\mathbf{x}')\,, \tag{5.9}$$

$$[\hat{\phi}(\mathbf{x},t),\hat{\phi}(\mathbf{x}',t)] = [\hat{\pi}(\mathbf{x},t),\hat{\pi}(\mathbf{x}',t)] = 0\,, \tag{5.10}$$

and the required Hermiticity properties:

$$\hat{\phi}^{\dagger}(\mathbf{x},t) = \hat{\phi}(\mathbf{x},t)\,, \qquad \hat{\pi}^{\dagger}(\mathbf{x},t) = \hat{\pi}(\mathbf{x},t)\,. \tag{5.11}$$

Unlike the Heisenberg picture, the operators of the field-coordinate ϕ and its canonically conjugate momentum π in the Schrödinger picture are time-independent, and from now on will be referred to by $\hat{\phi}(\mathbf{x})$ and $\hat{\pi}(\mathbf{x})$. In this picture, the canonically quantised form of (5.4) is defined on the hypersurface $t = 0$ as:

$$H_0[\hat{\phi},\hat{\pi}] = \frac{1}{2}\int d^3\mathbf{x}\,\left[\hat{\pi}^2(\mathbf{x}) + \hat{\phi}(\mathbf{x})\,(-\nabla^2 + m^2)\,\hat{\phi}(\mathbf{x})\right]. \tag{5.12}$$

The space of quantum states, namely Hilbert space, is an abstract physical space in which a physical state of a dynamical system in the Schrödinger picture is represented by a time-dependent ket-vector $|\Psi;t\rangle$. To give a concrete quantum mechanical wave description of these states together with the operators acting on them, we need to introduce a representation space of eigenvectors as the basis of Hilbert space so that by projecting the quantum states $|\Psi;t\rangle$ of the Hilbert space onto the basis-vectors, we obtain the quantum mechanical analogy of wave functions, namely the wave-functionals. For the field-configuration space representation, the basis-vectors in the Schrödinger picture are taken to be the time-independent eigenstates $|\varphi(\mathbf{x})\rangle$ of the Hermitian field operator $\hat{\phi}(\mathbf{x})$, defined on the quantisation surface $t = 0$ by the eigenvalue equation:

$$\hat{\phi}(\mathbf{x})\,|\varphi(\mathbf{x})\rangle = \varphi(\mathbf{x})\,|\varphi(\mathbf{x})\rangle\,, \tag{5.13}$$

with the eigenstates $|\varphi(\mathbf{x})\rangle$ being complete and orthonormal:

$$\langle\varphi(\mathbf{x})|\varphi_0(\mathbf{x})\rangle = \delta[\varphi-\varphi_0]\,, \qquad \int \mathcal{D}\varphi\,|\varphi(\mathbf{x})\rangle\langle\varphi(\mathbf{x})| = \mathbf{1}\,, \qquad \mathcal{D}\varphi = \prod_{\mathbf{x}} d\varphi(\mathbf{x})\,. \tag{5.14}$$

Here, the eigenvalue $\varphi(\mathbf{x})$ is a real function of the position coordinates $\mathbf{x} = (x_1, x_2, x_3)$, and $\mathbf{1}$ is the identity operator. In this φ-representation space, the physical state $|\Psi,t\rangle$ of the system is identified by a time-dependent wave-functional of the field eigenvalue $\varphi(\mathbf{x})$:

$$\langle\varphi|\Psi;t\rangle = \Psi[\varphi;t]\,, \tag{5.15}$$

and the inner product of any two quantum states, say at time $t = 0$, is defined through the functional integration as:

$$\langle \Psi_1 | \Psi_2 \rangle = \int \mathcal{D}\varphi \, \langle \Psi_1 | \varphi \rangle \langle \varphi | \Psi_2 \rangle = \int \mathcal{D}\varphi \, \Psi_1^*[\varphi] \, \Psi_2[\varphi] \,, \tag{5.16}$$

where $\Psi_1^*[\varphi] = \langle \Psi_1 | \varphi \rangle$ is the complex conjugate of $\langle \varphi | \Psi_1 \rangle$.

To find the φ-representation of the momentum operator $\pi(\mathbf{x})$ in the Schrödinger picture, we consider the matrix element $\langle \varphi | [\, \hat{\phi}(\mathbf{x}'), \hat{\pi}(\mathbf{x}) \,] | \varphi_0 \rangle$, giving with the help of (5.9), (5.13) and (5.14):

$$(\varphi - \varphi_0) \langle \varphi | \hat{\pi}(\mathbf{x}) | \varphi_0 \rangle = i\delta(\mathbf{x} - \mathbf{x}') \, \delta[\varphi - \varphi_0] \,. \tag{5.17}$$

Then, by making use of the fact that:

$$\frac{\delta}{\delta\varphi(\mathbf{x})} \Big[(\varphi(\mathbf{x}') - \varphi_0(\mathbf{x}')) \delta[\varphi - \varphi_0] \Big] = (\varphi - \varphi_0) \, \frac{\delta}{\delta\varphi(\mathbf{x})} \delta[\varphi - \varphi_0] + \delta(\mathbf{x} - \mathbf{x}') \, \delta[\varphi - \varphi_0] = 0 \,, \tag{5.18}$$

we obtain:

$$\langle \varphi | \hat{\pi}(\mathbf{x}) | \varphi_0 \rangle = -i \, \frac{\delta}{\delta\varphi(\mathbf{x})} \langle \varphi | \varphi_0 \rangle \,, \quad \Longrightarrow \quad \langle \varphi | \hat{\pi}(\mathbf{x}) = -i \, \frac{\delta}{\delta\varphi(\mathbf{x})} \langle \varphi | \,. \tag{5.19}$$

Now, the matrix element of a general function of the operators $\hat{\phi}$ and $\hat{\pi}$, denoted by $O(\hat{\phi}, \hat{\pi})$, can be expressed in the φ-space representation as:

$$\langle \varphi | O(\hat{\phi}, \hat{\pi}) | \varphi_0 \rangle = O(\varphi, -i \, \frac{\delta}{\delta\varphi}) \, \delta[\varphi - \varphi_0] \,. \tag{5.20}$$

Similarly, if $O(\hat{\phi}, \hat{\pi})$ is to operate on a physical state vector $|\Psi; t\rangle$ in this representation, we can safely write:

$$\langle \varphi | O(\hat{\phi}, \hat{\pi}) | \Psi; t \rangle = O(\varphi, -i \, \frac{\delta}{\delta\varphi}) \, \Psi[\varphi; t] \,. \tag{5.21}$$

Another useful representation space in the Schrödinger picture is the conjugate momentum space in which the basis-vectors of the physical states are the eigenstates $|\pi(\mathbf{x})\rangle$ of the Hermitian momentum operator $\hat{\pi}(\mathbf{x})$, defined by:

$$\hat{\pi}(\mathbf{x}) \, |\pi(\mathbf{x})\rangle = \pi(\mathbf{x}) \, |\pi(\mathbf{x})\rangle \,, \tag{5.22}$$

where the eigenvalue $\pi(\mathbf{x})$ is a real function of the position coordinates and the eigenstates satisfy the orthonormality and completeness relations:

$$\langle\pi(\mathbf{x})|\pi_0(\mathbf{x})\rangle = \delta'[\pi - \pi_0]\,, \qquad \int \mathcal{D}'\pi\ |\pi(\mathbf{x})\rangle\langle\pi(\mathbf{x})| = \mathbf{1}\,. \tag{5.23}$$

Here, the primed delta and the primed measure $\mathcal{D}'\pi$ denote:

$$\delta'[\pi - \pi_0] = \det(2\pi)\ \delta[\pi - \pi_0]\,, \qquad \mathcal{D}'\pi = \prod_{\mathbf{x}} \frac{d\pi(\mathbf{x})}{2\pi} = \det(1/2\pi)\ \mathcal{D}\pi\,, \tag{5.24}$$

with $\det(a)$ being a determinant of an infinite-dimensional diagonal matrix with all elements equal to $a \in \mathbb{C}$. The π-representation of the field operator $\hat{\phi}(\mathbf{x})$ can be achieved in exactly the same way that led to (5.19), giving:

$$\langle\pi|\hat{\phi}(\mathbf{x}) = i\frac{\delta}{\delta\pi(\mathbf{x})}\ \langle\pi|\,. \tag{5.25}$$

To establish a simple transformation relation between the φ-representation and the π-representation, we need to determine the basis product $\langle\varphi|\pi\rangle$ as an explicit functional of φ and π. This can be achieved by recalling the fact that $\langle\varphi|\pi\rangle$ is the solution of the first-order functional differential equation:

$$-i\frac{\delta}{\delta\varphi(\mathbf{x})}\ \langle\varphi|\pi\rangle = \pi(\mathbf{x})\ \langle\varphi|\pi\rangle\,, \tag{5.26}$$

deduced from $\langle\varphi|\hat{\pi}(\mathbf{x})|\pi\rangle$. This equation can be easily solved for $\langle\varphi|\pi\rangle$, giving the plane wave-functional solution:

$$\langle\varphi|\pi\rangle = \mathsf{c}\ \mathrm{e}^{i\int d\mathbf{x}\,\varphi(\mathbf{x})\pi(\mathbf{x})}\,, \tag{5.27}$$

where c is a normalization constant which can be determined from the orthonormality condition (5.14) as follows: consider writing $\langle\varphi|\varphi_0\rangle$ as

$$\langle\varphi|\varphi_0\rangle = \int \mathcal{D}'\pi\ \langle\varphi|\pi\rangle\langle\pi|\varphi_0\rangle = \delta[\varphi - \varphi_0]\,, \tag{5.28}$$

then by substituting (5.27) into (5.28) and using the δ-functional integral representation:

$$\delta[\varphi - \varphi_0] = \int \mathcal{D}'\pi\ \mathrm{e}^{i\int d\mathbf{x}\,[\varphi(\mathbf{x})-\varphi_0(\mathbf{x})]\pi(\mathbf{x})}\,, \tag{5.29}$$

we find that $c = 1$. Let us remark here that the factors of $\det(2\pi)$ and $\det(1/2\pi)$ in (5.23) have been chosen in this way so that (5.27) does not accommodate an infinite normalization factor. We can now show that the Schrödinger wave-functional in the π-representation,

$$\widetilde{\Psi}[\pi] = \langle \pi | \Psi \rangle \,, \tag{5.30}$$

is precisely the functional Fourier transform of $\Psi[\varphi]$. All we have to do to demonstrate this is rewriting $\langle \varphi | \Psi \rangle$ in the form:

$$\langle \varphi | \Psi \rangle = \langle \varphi | \mathbf{1} | \Psi \rangle = \int \mathcal{D}'\pi \; \langle \varphi | \pi \rangle \langle \pi | \Psi \rangle \,, \tag{5.31}$$

which implies the functional Fourier integral transformation:

$$\Psi[\varphi] = \int \mathcal{D}'\pi \; \mathrm{e}^{i \int d\mathbf{x}\, \varphi(\mathbf{x}) \pi(\mathbf{x})} \; \widetilde{\Psi}[\pi] \,. \tag{5.32}$$

The time evolution of the physical state $|\Psi; t\rangle$ of a dynamical system is described by the Schrödinger equation:

$$i \frac{\partial |\Psi; t\rangle}{\partial t} = H \, |\Psi; t\rangle \,, \tag{5.33}$$

where H denotes the quantised classical Hamiltonian of the system. If H is a time-independent, (5.33) has a simple formal solution:

$$|\Psi; t\rangle = \mathrm{e}^{-iH(t-t_0)} \, |\Psi; t_0\rangle \,. \tag{5.34}$$

In what follows, we shall restrict ourselves to the φ-representation space and to time-independent Hamiltonians only. Using the language of wave-functionals and Hamiltonians of the form $H[\hat{\phi}, \hat{\pi}]$, we represent the Schrödinger equation (5.33) and its solution (5.34) by:

$$i \frac{\partial \Psi[\varphi; t]}{\partial t} = H[\varphi, -i \, \frac{\delta}{\delta \varphi} \,] \, \Psi[\varphi; t] \,, \tag{5.35}$$

$$\Psi[\varphi; t] = \langle \varphi | \mathrm{e}^{-iH(t-t_0)} | \Psi; t_0 \rangle = \exp \left(-iH[\varphi, -i \, \frac{\delta}{\delta \varphi} \,](t - t_0) \right) \Psi[\varphi; t_0] \,. \tag{5.36}$$

Also, by using the completeness relation (5.14), we can express (5.36) as:

$$\Psi[\varphi;t] = \int \mathcal{D}\bar{\varphi}\ \langle\varphi|\mathrm{e}^{-iH(t-t_0)}|\bar{\varphi}\rangle\ \Psi[\bar{\varphi};t_0]\,. \tag{5.37}$$

It follows from (5.36) and (5.37) that if the state of the system is known at time t_0 its state at a later time $t > t_0$ can be determined. A simple illustrative example to consider is the special case in which the state of the system under analysis at a time t_0 is given by $\Psi[\varphi;t_0] = \mathtt{N}(t_0)\,\delta[\varphi - \varphi_0]$, where $\varphi_0(\mathbf{x})$ is a fixed field configuration and $\mathtt{N}(t_0)$ is an arbitrary function of t_0. In this case, (5.37) provide us with the wave-functional describing the system at time $t > t_0$, namely;

$$\Psi[\varphi;t] = \mathtt{N}(t_0)\ \langle\varphi|\mathrm{e}^{-iH(t-t_0)}|\,\varphi_0\rangle\,. \tag{5.38}$$

In this example, we can interpret $\Psi[\varphi;t]$ as the transition probability amplitude for the system to propagate from the initial field configuration $\varphi_0(\mathbf{x})$ at time t_0 to the field configuration $\varphi(\mathbf{x})$ at a later time t.

Since the Hamiltonian operator in (5.35) does not depend on time, we may use the separation of variables to separate out the time-dependent part of the wave-functional $\Psi[\varphi;t]$ from its stationary part, giving:

$$\Psi[\varphi;t] = \mathrm{e}^{-iEt}\ \Psi[\varphi]\,, \tag{5.39}$$

with the eigenfunctional $\Psi[\varphi] = \Psi[\varphi;0]$ satisfying the Schrödinger stationary state equation:

$$H[\varphi, -i\delta/\delta\varphi]\,\Psi[\varphi] = E\,\Psi[\varphi]\,, \tag{5.40}$$

where E is a constant energy eigenvalue. By analogy with the fundamental concepts of quantum mechanics, the expectation value of an observable $\mathtt{F}[\hat{\phi}(\mathbf{x}), \hat{\pi}(\mathbf{x})]$ is postulated as:

$$\langle\mathtt{F}\rangle = \int \mathcal{D}\varphi\ \Psi^*[\varphi;t]\,\mathtt{F}[\varphi, -i\delta/\delta\varphi]\,\Psi[\varphi;t]\,, \tag{5.41}$$

with the wave-functional being normalized to unity:

$$\int \mathcal{D}\varphi\ \big|\Psi[\varphi;t]\big|^2 = 1\,. \tag{5.42}$$

5.3 The Vacuum Functional For Free Scalar Fields

In this section, we shall consider the bosonic theory of a massive scalar field described by the classical free Hamiltonian (5.4), giving two different ways of calculating the exact Schrödinger vacuum functional for the system.

In the Schrödinger representation, the quantised version of the classical Hamiltonian in (5.4) is:

$$H_0[\varphi, -i\delta/\delta\varphi] = \frac{1}{2}\int d^3\mathbf{x}\,\left[-\frac{\delta^2}{\delta\varphi^2(\mathbf{x})} + \varphi(\mathbf{x})\,(-\nabla^2 + m^2)\,\varphi(\mathbf{x})\right]. \tag{5.43}$$

By substituting this into (5.40), we obtain the Schrödinger equation of the stationary wave-functionals $\Psi_{\mathtt{n}}[\varphi]$:

$$\frac{1}{2}\int d^3\mathbf{x}\,\left[-\frac{\delta^2\,\Psi_{\mathtt{n}}[\varphi]}{\delta\varphi^2(\mathbf{x})} + \varphi(\mathbf{x})\,(-\nabla^2 + m^2)\,\varphi(\mathbf{x})\Psi_{\mathtt{n}}[\varphi]\right] = E_{\mathtt{n}}\,\Psi_{\mathtt{n}}[\varphi]\,, \tag{5.44}$$

where $\mathtt{n}$ denotes the energy levels of the system. Now, our task is to solve (5.44) for the lowest energy eigenfunctional, namely the ground state or the vacuum wave-functional $\Psi_0[\varphi]$. One way to solve this functional equation is to reduce it to a set of ordinary differential equations such that the product of their solutions gives the required wave-functional solution. To achieve this goal, we first restrict the bosonic field system to a large cubic box of volume $\mathtt{V} = L^3$, and then introduce a set of an orthonormal basis:

$$\int_{\mathtt{V}} d^3\mathbf{x}\;\; u_n^*(\mathbf{x})\,u_m(\mathbf{x}) = \delta_{nm}\,, \qquad \sum_n^{\infty}\, u_n^*(\mathbf{x})\,u_n(\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y})\,, \tag{5.45}$$

such that $\varphi(\mathbf{x})$ can be expanded as:

$$\varphi(\mathbf{x}) = \sum_n^{\infty}\, q_n\,u_n(\mathbf{x})\,, \qquad q_n = \int_{\mathtt{V}} d^3\mathbf{x}\;\varphi(\mathbf{x})\,u_n^*(\mathbf{x})\,. \tag{5.46}$$

In the limiting process $L \to \infty$, the restriction on the field being in a finite spacial volume is removed. On this basis, we can represent the functional derivative as:

$$\frac{\delta}{\delta\varphi(\mathbf{x})} = \sum_n^{\infty}\, u_n^*(\mathbf{x})\,\frac{\partial}{\partial q_n}\,. \tag{5.47}$$

This expression clearly demonstrates the analogy with the d-dimensional gradient:

$$\nabla = \sum_{n=1}^{d} \hat{x}_n \frac{\partial}{\partial x_n}, \tag{5.48}$$

with $\hat{x}_n$ as a basis vector. An appropriate candidate for an orthonormal basis is the periodical Fourier set of complex eigenfunctions:

$$u_{\mathbf{n}}(\mathbf{x}) = \frac{1}{\sqrt{L^3}} \mathrm{e}^{i\mathbf{k_n}\cdot\mathbf{x}}, \quad \text{with} \quad \mathbf{k_n} = \frac{2\pi}{L}\mathbf{n}, \tag{5.49}$$

where $\mathbf{k_n} = (k_{n_1}, k_{n_2}, k_{n_3})$ and $\mathbf{n} = (n_1, n_2, n_3)$ such that

$$\mathbf{k_n}\cdot\mathbf{x} = \sum_{i=1}^{3} k_{n_i} x_i, \qquad k_{n_i} = \frac{2\pi}{L} n_i, \qquad n_i \in \mathbb{Z}. \tag{5.50}$$

Here, the range of each spacial coordinate x_i is defined by $-L/2 \leq x_i \leq L/2$. By using this basis in (5.46) and replacing q_n with $\widetilde{\varphi}(\mathbf{k_n})/\sqrt{L^3}$, we can write:

$$\varphi(\mathbf{x}) = \frac{1}{L^3} \sum_{\mathbf{n}=-\infty}^{\infty} \widetilde{\varphi}(\mathbf{k_n})\, \mathrm{e}^{i\mathbf{k_n}\cdot\mathbf{x}}, \qquad \widetilde{\varphi}(\mathbf{k_n}) = \int_{\mathrm{V}} d^3\mathbf{x}\, \varphi(\mathbf{x})\, \mathrm{e}^{-i\mathbf{k_n}\cdot\mathbf{x}}, \tag{5.51}$$

where

$$\widetilde{\varphi}^*(\mathbf{k_n}) = \widetilde{\varphi}(-\mathbf{k_n}), \qquad \mathbf{k}_{-\mathbf{n}} = -\mathbf{k_n}, \qquad \sum_{\mathbf{n}=-\infty}^{\infty} = \prod_{i=1}^{3} \sum_{n_i=-\infty}^{\infty}. \tag{5.52}$$

Also, from (5.47) it follows that:

$$\frac{\delta}{\delta\varphi(\mathbf{x})} = \sum_{\mathbf{n}=-\infty}^{\infty} \mathrm{e}^{-i\mathbf{k_n}\cdot\mathbf{x}} \frac{\partial}{\partial\, \widetilde{\varphi}(\mathbf{k_n})}. \tag{5.53}$$

Note that in the continuum limit $L \to \infty$, the volume of the small cubic cells $\triangle\mathbf{k_n} = (2\pi)^3/L^3$ in the $\mathbf{k_n}$-lattice space tend to zero and $L^{-3}\sum = (2\pi)^{-3}\sum \triangle\mathbf{k_n} \to \int d^3\mathbf{k}/(2\pi)^3$

in which case the field φ in (5.51) and its partial derivative [1] (5.53) change to:

$$\varphi(\mathbf{x}) = \int_{\mathbb{R}^3} \frac{d^3\mathbf{k}}{(2\pi)^3}\ \widetilde{\varphi}(\mathbf{k})\ \mathrm{e}^{i\mathbf{k}.\mathbf{x}}\,, \qquad \frac{\delta}{\delta\varphi(\mathbf{x})} = \int_{\mathbb{R}^3} d^3\mathbf{k}\ \mathrm{e}^{-i\mathbf{k}.\mathbf{x}}\ \frac{\delta}{\delta\,\widetilde{\varphi}(\mathbf{k})}\,. \tag{5.54}$$

On the $\mathbf{k_n}$-lattice space, the vacuum wave-functional $\Psi_0[\varphi]$, with φ given by (5.51), is represented as:

$$\Psi_0[\varphi] \equiv \overline{\Psi}_0\big(\{\widetilde{\varphi}(\mathbf{k_n})\}_{\mathbf{n}\in\mathbb{Z}^3}\big)\,, \qquad \{\widetilde{\varphi}(\mathbf{k_n})\}_{\mathbf{n}\in\mathbb{Z}^3} = \{\widetilde{\varphi}(k_{n_1}, k_{n_2}, k_{n_3})\}_{(n_1,n_2,n_3)\in\mathbb{Z}^3}\,, \tag{5.55}$$

and the Hamiltonian (5.43) takes the form:

$$H_0 = -\frac{1}{2}\sum_{\mathbf{n}=-\infty}^{\infty}\Big[\frac{\partial}{\partial\,\phi(\mathbf{k_n})}\,\frac{\partial}{\partial\,\phi(-\mathbf{k_n})} - \omega^2(\mathbf{k_n})\,\phi(\mathbf{k_n})\,\phi(-\mathbf{k_n})\Big]\,, \tag{5.56}$$

where

$$\phi(\mathbf{k_n}) = \widetilde{\varphi}(\mathbf{k_n})/\sqrt{L^3}\,, \qquad \omega(\mathbf{k_n}) = \sqrt{\mathbf{k}_\mathbf{n}^2 + m^2}\,. \tag{5.57}$$

By making the change of variables:

$$\phi(\mathbf{k_n}) = \mathcal{X}(\mathbf{k_n})\ \mathrm{e}^{i\theta(\mathbf{k_n})}\,, \quad \text{such that} \quad \frac{\partial}{\partial\phi(\mathbf{k_n})} = \mathrm{e}^{-i\theta(\mathbf{k_n})}\ \frac{\partial}{\partial\mathcal{X}(\mathbf{k_n})}\,, \tag{5.58}$$

where $\mathcal{X}(\mathbf{k_n}) = \mathcal{X}(-\mathbf{k_n})$ and $\theta(-\mathbf{k_n}) = -\theta(\mathbf{k_n})$ so that $\phi^*(\mathbf{k_n}) = \phi(-\mathbf{k_n})$, we can express (5.56) as a denumerably infinite system of uncoupled harmonic oscillators:

$$H_0(\{\mathcal{X}_\mathbf{n}\}_{\mathbf{n}\in\mathbb{Z}^3}) = \sum_{\mathbf{n}=-\infty}^{\infty} h(\mathcal{X}_\mathbf{n})\,, \tag{5.59}$$

[1] In the continuum limit $L \to \infty$, the partial derivative with respect to $\widetilde{\varphi}(\mathbf{k_n})$ in (5.53) should be changed according to:

$$\frac{L^3}{(2\pi)^3}\,\frac{\partial}{\partial\,\widetilde{\varphi}(\mathbf{k_n})} \to \frac{\delta}{\delta\,\widetilde{\varphi}(\mathbf{k})}\,,$$

so that we maintain the consistency between the Kronecker delta $\delta_{\mathbf{k_n}\mathbf{k_{n'}}}$ defined on the lattice and its counterpart $\delta(\mathbf{k}-\mathbf{k}')$ in the continuum space, which are related by the correspondence:

$$\frac{L^3}{(2\pi)^3}\,\delta_{\mathbf{k_n}\mathbf{k_{n'}}} = \frac{L^3}{(2\pi)^3}\,\frac{\partial\widetilde{\varphi}(\mathbf{k_{n'}})}{\partial\,\widetilde{\varphi}(\mathbf{k_n})} \Longleftrightarrow \delta(\mathbf{k}-\mathbf{k}') = \frac{\delta\widetilde{\varphi}(\mathbf{k}')}{\delta\,\widetilde{\varphi}(\mathbf{k})}\,.$$

Some authors like B. Hatfield prefer to define $\delta/\delta\varphi(\mathbf{x})$ in (5.54) with the measure $d^3\mathbf{k}/(2\pi)^3$ instead. This convention, however, requires the definition:

$$\frac{\delta\widetilde{\varphi}(\mathbf{k}')}{\delta\,\widetilde{\varphi}(\mathbf{k})} = (2\pi)^3\,\delta(\mathbf{k}-\mathbf{k}')\,.$$

where

$$h(\mathcal{X}_{\mathbf{n}}) = -\frac{1}{2}\frac{\partial^2}{\partial \mathcal{X}_{\mathbf{n}}^2} + \frac{1}{2}\omega_{\mathbf{n}}^2 \mathcal{X}_{\mathbf{n}}^2, \qquad \mathcal{X}_{\mathbf{n}} = \mathcal{X}(\mathbf{k}_{\mathbf{n}}), \qquad \omega_{\mathbf{n}} = \omega(\mathbf{k}_{\mathbf{n}}). \tag{5.60}$$

Here $h(\mathcal{X}_{\mathbf{n}})$ is exactly the Hamiltonian of the one-dimensional harmonic oscillator whose ground state eigenfunction $\psi(\mathcal{X}_{\mathbf{n}})$ and energy ε_0 are given by:

$$\psi(\mathcal{X}_{\mathbf{n}}) = (\omega_{\mathbf{n}}/\pi)^{1/4}\ \mathrm{e}^{-\omega_{\mathbf{n}}\mathcal{X}_{\mathbf{n}}^2/2}, \qquad \varepsilon_0 = \frac{1}{2}\omega_{\mathbf{n}}. \tag{5.61}$$

Now a separation of variables is possible to apply to the Schrödinger equation with the Hamiltonian (5.59), and therefore the lowest energy state solution can be expressed as a multiple of the ground state eigenfunctions $\{\psi(\mathcal{X}_{\mathbf{n}})\}$:

$$\overline{\Psi}_0 = \prod_{\mathbf{n}=-\infty}^{\infty} \psi(\mathcal{X}_{\mathbf{n}}) = \Big[\prod_{\mathbf{n}=-\infty}^{\infty} (\omega_{\mathbf{n}}/\pi)^{1/4}\Big] \exp\Big(-\frac{1}{2}\sum_{\mathbf{n}=-\infty}^{\infty} \omega_{\mathbf{n}}\mathcal{X}_{\mathbf{n}}^2\Big), \tag{5.62}$$

where $\prod_{\mathbf{n}=-\infty}^{\infty} = \prod_{n_1=-\infty}^{\infty}\prod_{n_2=-\infty}^{\infty}\prod_{n_3=-\infty}^{\infty}$. By using the first relation in (5.57) and (5.58), we can rewrite $\overline{\Psi}_0$ in terms of the Fourier coefficients $\widetilde{\varphi}(\mathbf{k}_{\mathbf{n}})$ as:

$$\overline{\Psi}_0 = \Big[\prod_{\mathbf{n}=-\infty}^{\infty} (\omega_{\mathbf{n}}/\pi)^{1/4}\Big] \exp\Big(-\frac{1}{2L^3}\sum_{\mathbf{n}=-\infty}^{\infty} \omega(\mathbf{k}_{\mathbf{n}})\,\widetilde{\varphi}(\mathbf{k}_{\mathbf{n}})\,\widetilde{\varphi}(-\mathbf{k}_{\mathbf{n}})\Big). \tag{5.63}$$

In the limit $L \to \infty$, the restriction on the scalar field system being enclosed in a large box of volume L^3 is removed, and the required vacuum functional in the $\widetilde{\varphi}$-configuration space is obtained as:

$$\overline{\Psi}_0[\widetilde{\varphi}] = \mathcal{N} \exp\Big(-\frac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\,\omega(\mathbf{k})\,\widetilde{\varphi}(\mathbf{k})\,\widetilde{\varphi}(-\mathbf{k})\Big), \tag{5.64}$$

with $\mathcal{N}$ being a normalisation constant independent of $\widetilde{\varphi}$:

$$\mathcal{N} = \prod_{\mathbf{n}=-\infty}^{\infty} (\omega(\mathbf{k}_{\mathbf{n}})/\pi)^{1/4}. \tag{5.65}$$

By substituting the Fourier transform of $\varphi(\mathbf{x})$:

$$\widetilde{\varphi}(\mathbf{k}) = \int d^3\mathbf{x}\ \varphi(\mathbf{x})\,\mathrm{e}^{-i\mathbf{k}.\mathbf{x}}, \tag{5.66}$$

into (5.64), we obtain the vacuum functional in the φ-configuration space:

$$\Psi_0[\varphi] = \mathcal{N} \exp\Big(-\frac{1}{2} \int d^3\mathbf{x}\, d^3\mathbf{y}\ \ \varphi(\mathbf{x})\, G_0(\mathbf{x},\mathbf{y})\, \varphi(\mathbf{y}) \Big)\,, \tag{5.67}$$

where

$$G_0(\mathbf{x},\mathbf{y}) = (-\nabla^2 + m^2)^{1/2}\, \delta(\mathbf{x}-\mathbf{y})\,. \tag{5.68}$$

In quantum field theoretic Schrödinger representation, the normalisation constant $\mathcal{N}$ of the vacuum functional is usually infinite, but irrelevant to physical results. This is because it cancels out in the computations of the expectation values. For example, consider the expectation value of an observable $\mathrm{F}[\hat{\phi}(\mathbf{x}), \hat{\pi}(\mathbf{x})]$:

$$\langle \mathrm{F} \rangle = \frac{\int \mathcal{D}\varphi\ \Psi_0^*[\varphi]\, \mathrm{F}[\varphi, -i\delta/\delta\varphi]\, \Psi_0[\varphi]}{\int \mathcal{D}\varphi\ \Psi_0^*[\varphi]\, \Psi_0[\varphi]}\,. \tag{5.69}$$

Since $\mathcal{N}$ is independent of φ and $\Psi_0[\varphi] = \mathcal{N}\,\Psi[\varphi]$, where $\Psi[\varphi]$ is the non-normalised wave-functional, we can simply take the $\mathcal{N}$'s in the numerator and denominator in (5.69) outside the integration sign and cancel them. The energy eigenvalue E_0 of the vacuum functional also suffers from a divergence. This is because, it is the sum of all the zero-point energies of the infinite number of the uncoupled harmonic oscillators describing the scalar field system:

$$\begin{aligned} E_0 &= \sum_{\mathbf{n}=-\infty}^{\infty} \frac{1}{2}\ \omega(\mathbf{k_n}) = \frac{1}{2}\,\delta(0) \int d^3\mathbf{k}\, \sqrt{\mathbf{k}^2 + m^2} \\ &= 2\pi\,\delta(0) \int_0^\infty dk\ k^2\, \sqrt{k^2+m^2}\,, \qquad \delta(0) = \lim_{L\to\infty} \frac{L^3}{(2\pi)^3}\,. \end{aligned} \tag{5.70}$$

Here, E_0 is infrared infinite because of the volume factor $\delta(0)$, and ultraviolet infinite because of the divergence of the defining integral (5.70) at high momenta. This infinite energy constant is usually eliminated by normal ordering, which modifies the original Hamiltonian H_0 in such away that $H_0 \to H_0 - \langle 0|H_0|0\rangle$, where $|0\rangle$ denotes the normalised vacuum state. Redefining the Hamiltonian in this way is harmless because experiments can only measure energy differences from the energy ground state but not the absolute energy values.

Another way to derive the vacuum functional in the Schrödinger representation is by introducing creation and annihilation operators $\hat{a}^\dagger(\mathbf{k})$ and $\hat{a}(\mathbf{k})$ respectively, and then

defining the vacuum in Fock space, just like in quantum mechanics, by $\hat{a}(\mathbf{k})|0\rangle = 0$ with $\langle 0|0\rangle = 1$. To illustrate this method, we begin by writing $\hat{a}(\mathbf{k})$ and $\hat{a}^\dagger(\mathbf{k})$ as:

$$\hat{a}(\mathbf{k}) = \frac{1}{\sqrt{2}} \int d^3\mathbf{x}\, e^{-i\mathbf{k}.\mathbf{x}} \left[\omega^{1/2}(\mathbf{k})\, \hat{\phi}(\mathbf{x}) + i\, \omega^{-1/2}(\mathbf{k})\, \hat{\pi}(\mathbf{x})\right], \tag{5.71}$$

$$\hat{a}^\dagger(\mathbf{k}) = \frac{1}{\sqrt{2}} \int d^3\mathbf{x}\, e^{i\mathbf{k}.\mathbf{x}} \left[\omega^{1/2}(\mathbf{k})\, \hat{\phi}(\mathbf{x}) - i\, \omega^{-1/2}(\mathbf{k})\, \hat{\pi}(\mathbf{x})\right]. \tag{5.72}$$

These are obtained from the two conjugate expressions (5.6) and (5.8) for $t = 0$ by simply solving for $a(\mathbf{k})$ and $a^*(\mathbf{k})$, and then turning them to operators satisfying the commutation relations:

$$[\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{p})] = (2\pi)^3\, \delta(\mathbf{k} - \mathbf{p}), \tag{5.73}$$

$$[\hat{a}(\mathbf{k}), \hat{a}(\mathbf{p})] = [\hat{a}^\dagger(\mathbf{k}), \hat{a}^\dagger(\mathbf{p})] = 0, \tag{5.74}$$

which can be verified by (5.9) and (5.10). We can now use these ladder operators to reformulate the Hamiltonian (5.12) as:

$$\begin{aligned} H_0 &= \frac{1}{2} \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, \omega(\mathbf{k}) \left(\hat{a}^\dagger(\mathbf{k})\, \hat{a}(\mathbf{k}) + \hat{a}(\mathbf{k})\, \hat{a}^\dagger(\mathbf{k})\right) \\ &= \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, \omega(\mathbf{k}) \left(\hat{a}^\dagger(\mathbf{k})\, \hat{a}(\mathbf{k}) + \frac{1}{2}\, [\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k})]\right). \end{aligned} \tag{5.75}$$

Here, the second term gives the divergent ground state energy in (5.70) which we usually eradicate by normal ordering. In simple terms, normal ordering means that all creation operators are to be placed to the left of annihilation operators. Under this scheme of operator ordering, (5.75) becomes:

$$H_0 = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, \omega(\mathbf{k})\, \hat{a}^\dagger(\mathbf{k})\, \hat{a}(\mathbf{k}). \tag{5.76}$$

In the Schrödinger formalism, the ladder operators in the φ-basis representation are given by:

$$\hat{a}(\mathbf{k}) = \frac{1}{\sqrt{2}} \int d^3\mathbf{x}\, e^{-i\mathbf{k}.\mathbf{x}} \left[\, \omega^{1/2}(\mathbf{k})\, \varphi(\mathbf{x}) + \omega^{-1/2}(\mathbf{k})\, \frac{\delta}{\delta\varphi(\mathbf{x})} \,\right], \tag{5.77}$$

$$\hat{a}^\dagger(\mathbf{k}) = \frac{1}{\sqrt{2}} \int d^3\mathbf{x}\, e^{i\mathbf{k}.\mathbf{x}} \left[\, \omega^{1/2}(\mathbf{k})\, \varphi(\mathbf{x}) - \omega^{-1/2}(\mathbf{k})\, \frac{\delta}{\delta\varphi(\mathbf{x})} \,\right]. \tag{5.78}$$

By analogy with quantum mechanics, we shall now show how to obtain the vacuum functional from the property $\hat{a}(\mathbf{k})|0\rangle = 0$. This requires considering:

$$\langle\varphi|\hat{a}(\mathbf{k})|0\rangle = \frac{1}{\sqrt{2}}\int d^3\mathbf{x}\, \mathrm{e}^{-i\mathbf{k}.\mathbf{x}}\left[\omega^{1/2}(\mathbf{k})\,\varphi(\mathbf{x}) + \omega^{-1/2}(\mathbf{k})\,\frac{\delta}{\delta\varphi(\mathbf{x})}\right]\Psi_0[\varphi] = 0\,, \qquad (5.79)$$

rather than the Schrödinger equation. To simplify this functional equation, we rewrite it in terms of the Fourier transform of $\varphi(\mathbf{x})$ using (5.54). In this way, we obtain the simple form:

$$\left[\frac{\omega(\mathbf{k})}{(2\pi)^3}\;\widetilde{\varphi}(\mathbf{k}) + \frac{\delta}{\delta\widetilde{\varphi}(-\mathbf{k})}\right]\overline{\Psi}_0[\widetilde{\varphi}] = 0\,, \qquad (5.80)$$

where $\overline{\Psi}_0[\widetilde{\varphi}] = \Psi_0[\varphi]$ for any φ given by (5.54). By analogy with the ordinary differential equation of first order:

$$(a\,x + \frac{d}{dx})\psi(x) = 0\,, \qquad (5.81)$$

which has a Gaussian solution:

$$\psi(x) = \mathrm{e}^{-a\,x^2/2}\,, \qquad a \in \mathbb{R}\,, \qquad (5.82)$$

we can easily deduce the vacuum functional solution of (5.80), giving:

$$\overline{\Psi}_0[\widetilde{\varphi}] = \mathcal{N}\,\exp\Big(-\frac{1}{2}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\,\omega(\mathbf{k})\,\widetilde{\varphi}(\mathbf{k})\,\widetilde{\varphi}(-\mathbf{k})\Big)\,, \qquad (5.83)$$

which is the same expression as (5.64). Here, the constant $\mathcal{N}$ is determined from the normalisation condition $\int \mathcal{D}'\widetilde{\varphi}\;\;\overline{\Psi}_0^*[\widetilde{\varphi}]\;\overline{\Psi}_0[\widetilde{\varphi}] = 1$, and found to have the same value of (5.65) as it should do. As for the excited states, they can be constructed by applying the creation operator $\hat{a}^\dagger(\mathbf{k})$ to the vacuum wave functional just like in quantum mechanics.

5.4 Vacuum Functionals and Path integrals

In this section, we shall show that the functional solutions of the Schrödinger equation for a scalar field have a path integral representation in which the limits of the functional integrals over the fields, defining the surface boundary conditions, are the argument of these functional solutions. In particular, we shall build a functional integral representation for the Schrödinger vacuum $\Psi_0[\varphi]$ in such a way that makes the φ-dependence more

explicit, i.e. appearing in the functional integrand as a source field rather than in the limits of integration as a boundary condition.

To illustrate this, we begin by considering the matrix element:

$$K[\varphi, \varphi_0; \triangle t] = \langle \varphi | \, \mathrm{e}^{-iH\triangle t} \, | \varphi_0 \rangle \,, \qquad \triangle t = t - t_0 \,, \tag{5.84}$$

defining the probability amplitude (the propagation kernel) for the transition from the field configuration $\varphi_0(\mathbf{x})$ at a time t_0 to its counterpart $\varphi(\mathbf{x})$ at a later time t. Here, H is a time-independent Hamiltonian of the form $H[\hat{\phi}, \hat{\pi}]$. Note that in the limit $\triangle t \to 0$ the propagator $K[\varphi, \varphi_0; \triangle t]$, as is also called, tends to $\delta[\varphi - \varphi_0]$. Now, let us show that this propagator is a solution to the Schrödinger functional equation (5.35). By differentiating (5.84) with respect to t, we have:

$$\frac{\partial}{\partial t} K[\varphi, \varphi_0; \triangle t] = -i \, \langle \varphi | H[\hat{\phi}, \hat{\pi}] \; \mathrm{e}^{-iH\triangle t} \, | \varphi_0 \rangle \,. \tag{5.85}$$

Then, by making use of the identity:

$$\langle \varphi | H[\hat{\phi}, \hat{\pi}] = H[\varphi, -i\frac{\delta}{\delta \varphi}] \, \langle \varphi | \,, \tag{5.86}$$

we complete our proof, showing the Schrödinger equation being satisfied by the propagator $K[\varphi, \varphi_0; \triangle t]$, i.e.

$$i \, \frac{\partial}{\partial t} \, K[\varphi, \varphi_0; \triangle t] = H[\varphi, -i\frac{\delta}{\delta \varphi}] \, K[\varphi, \varphi_0; \triangle t] \,. \tag{5.87}$$

According to Feynman path integral approach [60], the propagator solution $K[\varphi, \varphi_0; \triangle t]$ to the Schrödinger equation, known also as the Schrödinger functional, can be represented as:

$$K[\varphi, \varphi_0; \triangle t] = \int_{\varphi_0}^{\varphi} \mathcal{D}\phi \int \mathcal{D}'\pi \, \exp\left(i \int_{t_0}^{t} dt' \int_{\mathbb{R}^3} d^3\mathbf{x} \left[\pi(\mathbf{x}, t') \dot{\phi}(\mathbf{x}, t') - \mathcal{H} \right] \right) , \tag{5.88}$$

with the surface boundary conditions $\phi(\mathbf{x}, t_0) = \varphi_0(\mathbf{x})$ and $\phi(\mathbf{x}, t) = \varphi(\mathbf{x})$, a time $\triangle t$ apart, being the argument of $K[\varphi, \varphi_0; \triangle t]$. Here, $\mathcal{H}$ denotes the Hamiltonian density which is a function of the classical field ϕ and its momentum conjugate π. Recall that the integration measures $\mathcal{D}\phi$ and $\mathcal{D}'\pi$ in (5.88) are, unlike those identified in (5.14) and

(5.24), defined over time-dependent fields:

$$\mathcal{D}\phi = \prod_{t_0<t'<t} \prod_{\mathbf{x}} d\phi(\mathbf{x},t')\,, \qquad \mathcal{D}'\pi = \det(1/2\pi) \prod_{t_0\leq t'\leq t} \prod_{\mathbf{x}} d\pi(\mathbf{x},t')\,. \tag{5.89}$$

For $\mathcal{H}(\phi,\pi)$ being quadratic in π, we can easily integrate out the π-dependence in (5.88), giving:

$$K[\varphi,\varphi_0;\triangle t] = \mathcal{N}\int_{\varphi_0}^{\varphi}\mathcal{D}\phi\ \mathrm{e}^{iS[\phi]}\,, \tag{5.90}$$

where $S[\phi]$ is the classical action of the scalar field system in Minkowski space-time, and $\mathcal{N}$ is the value of the functional integration over π which is a constant independent of ϕ.

Now let us define a complete orthonormal set of eigenstates $|E_n\rangle = |n\rangle \equiv |\Psi_n\rangle$ for the Hamiltonian $H[\hat{\phi},\hat{\pi}]$ under consideration:

$$\sum_{n=0}^{\infty} |E_n\rangle\langle E_n| = \mathbf{1}\,, \qquad \langle E_m|E_n\rangle = \delta_{mn}\,, \tag{5.91}$$

where E_n is a discrete energy eigenvalue of $H[\hat{\phi},\hat{\pi}]$. To extract the Schrödinger vacuum functional $\Psi_0[\varphi]$ from $K[\varphi,\varphi_0;\triangle t]$, we insert the series of the complete eigenstates $|E_n\rangle$ between the field brakets in (5.84) to obtain:

$$K[\varphi,\varphi_0;\triangle t] = \langle\varphi|\mathrm{e}^{-iH\triangle t}\,\mathbf{1}|\,\varphi_0\rangle = \sum_{n=0}^{\infty}\Psi_n[\varphi]\ \Psi_n^*[\varphi_0]\ \mathrm{e}^{-iE_n\triangle t}\,. \tag{5.92}$$

Multiplying both sides of (5.92) with $\mathrm{e}^{iE_0\triangle t}$, recalling that $E_n - E_0 > 0$ for all $n \neq 0$, and then taking the limit as $\triangle t \to -i\infty$ gives:

$$\Psi_0[\varphi]\ \Psi_0^*[\varphi_0] = \lim_{\triangle t\to -i\infty}\left(\mathrm{e}^{iE_0\triangle t}\,K[\varphi,\varphi_0;\triangle t]\right). \tag{5.93}$$

For simplicity, if we allow the constant field configuration $\varphi_0(\mathbf{x})$, describing the surface boundary at t_0 in the path integral formalism, to vanish and use the functional integral expression (5.90) in (5.93) we arrive at:

$$\Psi_0[\varphi] = \mathcal{N}_0 \lim_{\triangle t\to -i\infty}\left(\mathrm{e}^{iE_0\triangle t}\,K[\varphi,0;\triangle t]\right) = \mathcal{N}_1 \lim_{\triangle t\to -i\infty}\int_0^{\varphi}\mathcal{D}\phi\ \mathrm{e}^{i(S[\phi]+E_0\triangle t)}, \tag{5.94}$$

where $\mathcal{N}_0 = 1/\Psi_0^*[0]$, and $\mathcal{N}_1 = \mathcal{N}\,\mathcal{N}_0$. The latter can be determined from the normaliza-

tion condition (5.42).

An alternative and more practical formulation of $\Psi_0[\varphi]$ can be obtained by considering the ratio $K[\varphi,\varphi_0;T]/K[\varphi_0,\varphi_0;T]$ for $\varphi_0=0$, which we can rewrite as:

$$\frac{K[\varphi,0;T]}{K[0,0;T]}=\frac{\Psi_0[\varphi]+a_1\,\Psi_1[\varphi]\,\mathrm{e}^{-i\triangle E_1T}+\cdots+a_n\,\Psi_n[\varphi]\,\mathrm{e}^{-i\triangle E_nT}+\ldots}{\Psi_0[0]+a_1\,\Psi_1[0]\,\mathrm{e}^{-i\triangle E_1T}+\cdots+a_n\,\Psi_n[0]\,\mathrm{e}^{-i\triangle E_nT}+\ldots}\,, \tag{5.95}$$

where $a_n=\Psi_n^*[0]/\Psi_0^*[0]$ with $\Psi_0[0]\neq 0$, $\triangle E_n=E_n-E_0>0$ and $T=\triangle t$. In the limit as T tends to $-i\infty$, we obtain:

$$\Psi_0[\varphi]=\lim_{T\to -i\infty}\frac{K[\varphi,0;T]}{K[0,0;T]}\,. \tag{5.96}$$

Here, we have chosen $\Psi_0[0]=1$. This is harmless indeed since $\Psi_0[\varphi]$ will be normalized eventually according to the normalization condition $\int\mathcal{D}\varphi\,|\Psi_0[\varphi]|^2=1$.

As for the energy eigenvalue E_0 associated with the vacuum functional $\Psi_0[\varphi]$, it is not difficult to deduce from expansion (5.92), giving:

$$E_0=-\lim_{\triangle\tau\to\infty}\left(\frac{1}{\triangle\tau}\,\ln K[\varphi,\varphi_0;-i\triangle\tau]\right), \tag{5.97}$$

where $\tau=it$ is the Euclidean time. At this stage, we can see that the Schrödinger propagation kernel $K[\varphi,\varphi_0;\triangle t]$ as well as the wave-functional $\Psi_0[\varphi]$ lead to the concept of a quantum field theory on a manifold with boundaries.

In what follows, we shall introduce a useful technique for making the φ-dependence of $\Psi_0[\varphi]$ more explicit in the path integral representation, i.e. appearing in the functional integrand as a source field rather than in the limits of integration as a boundary condition. We begin by defining an eigenbra $\langle\varphi_{\mathtt{D}}|$ with the property of being annihilated by the field operator $\hat{\phi}(\mathbf{x})$, i.e. $\langle\varphi_{\mathtt{D}}|=\langle\varphi=0|$ such that $\langle\varphi_{\mathtt{D}}\,|\hat{\phi}(\mathbf{x})=0$. From (5.27), it follows that:

$$\langle\varphi_{\mathtt{D}}|\pi\rangle=\mathrm{e}^{i\int d\mathbf{x}\,\varphi_{\mathtt{D}}(\mathbf{x})\pi(\mathbf{x})}=1\,. \tag{5.98}$$

Here the subscript $\mathtt{D}$ in $\varphi_{\mathtt{D}}$ stands for Dirichlet because we shall show later that the null field $\varphi_{\mathtt{D}}(\mathbf{x})$ will correspond to Dirichlet conditions on both surface boundaries in the functional integral representation of $\Psi_0[\varphi]$. Now, the φ-dependence of any eigenbra $\langle\varphi|$ of the field

operator $\hat{\phi}(\mathbf{x})$ can be made explicit by writing:

$$\langle\varphi| = \langle\varphi_{\mathrm{D}}|\, \mathrm{e}^{i\int d\mathbf{x}\,\varphi(\mathbf{x})\,\hat{\pi}(\mathbf{x})}\,, \tag{5.99}$$

such that $\frac{\delta}{\delta\varphi(\mathbf{x})}\,\langle\varphi| = i\,\langle\varphi|\hat{\pi}(\mathbf{x})$. By virtue of the commutation relation $[\hat{\phi}(\mathbf{x}), \hat{\pi}(\mathbf{x}')] = i\delta(\mathbf{x}-\mathbf{x}')$, we can easily show that:

$$\langle\varphi_{\mathrm{D}}|\hat{\phi}(\mathbf{x}') = \langle\varphi|\, \mathrm{e}^{-i\int d\mathbf{x}\,\varphi(\mathbf{x})\,\hat{\pi}(\mathbf{x})}\;\hat{\phi}(\mathbf{x}') = 0\,. \tag{5.100}$$

In (5.90), we have shown that $K[\varphi, \varphi_0; \triangle t]$ is given by a functional integral over field configurations $\phi(\mathbf{x}, t)$ subject to the boundary conditions $\phi(\mathbf{x}, t_0) = \varphi_0(\mathbf{x})$ and $\phi(\mathbf{x}, t) = \varphi(\mathbf{x})$. Now, we shall reformulate (5.90) such that the arguments of $K[\varphi, \varphi_0; \triangle t]$, and accordingly $\Psi_0[\varphi]$, are no longer acting as boundary conditions but as source terms. To show this we begin by substituting (5.99) into (5.84), giving:

$$K[\varphi, \varphi_0; T] = \langle\varphi_{\mathrm{D}}|\, \mathrm{e}^{i\int d\mathbf{x}\,\varphi(\mathbf{x})\,\hat{\pi}(\mathbf{x})}\; \mathrm{e}^{-iHT}\, \mathrm{e}^{-i\int d\mathbf{x}\,\varphi_0(\mathbf{x})\,\hat{\pi}(\mathbf{x})}|\varphi_{\mathrm{D}}\rangle\,. \tag{5.101}$$

In order to make our subsequent argument clearer, we shall pause for a moment to briefly review the Dirac picture and its relation with the Schrödinger and Heisenberg pictures. Consider a quantum field theory (in 4-dimensional Minkowski space-time) described in Schrödinger picture by the time-independent Hamiltonian:

$$\overline{\mathbf{H}}_{\mathrm{S}} = H_{\mathrm{S}} + V_{\mathrm{S}}\,, \qquad H_{\mathrm{S}} = \int_{\mathbb{R}^3} d^3\mathbf{x}\;\mathcal{H}(\hat{\phi}_{\mathrm{S}}, \hat{\pi}_{\mathrm{S}})\,, \qquad V_{\mathrm{S}} = \int_{\mathbb{R}^3} d^3\mathbf{x}\;\mathcal{V}(\hat{\phi}_{\mathrm{S}}, \hat{\pi}_{\mathrm{S}})\,, \tag{5.102}$$

where $\hat{\phi}_{\mathrm{S}} = \hat{\phi}(\mathbf{x}, 0)$ and $\hat{\pi}_{\mathrm{S}} = \hat{\pi}(\mathbf{x}, 0)$. Here, H_{S} is the part of the full Hamiltonian $\overline{\mathbf{H}}_{\mathrm{S}}$ for which we know how to solve the corresponding equation of motion and V_{S} is a perturbing interaction. In Schrödinger picture, referred to by the subscript S, the quantum states evolve with time, i.e. $|\Psi; t\rangle_{\mathrm{S}} = \mathrm{e}^{i\overline{\mathbf{H}}_{\mathrm{S}}\,t}|\Psi\rangle_{\mathrm{S}}$, whereas the operators and the basis vectors, e.g. $|\varphi\rangle_{\mathrm{S}}$, remain stationary. By contrast, the states in the Heisenberg pictures are time-independent, i.e. $|\Psi\rangle_{\mathrm{H}} = |\Psi\rangle_{\mathrm{S}}$, while the operators and the basis vectors evolve according to:

$$\hat{A}_{\mathrm{H}}(\mathbf{x}, t) = \mathrm{e}^{i\overline{\mathbf{H}}_{\mathrm{S}}t}\;\hat{A}_{\mathrm{S}}(\mathbf{x})\;\mathrm{e}^{-i\overline{\mathbf{H}}_{\mathrm{S}}t}\,, \qquad |\chi; t\rangle_{\mathrm{H}} = \mathrm{e}^{-i\overline{\mathbf{H}}_{\mathrm{S}}t}\,|\chi\rangle_{\mathrm{S}}\,, \tag{5.103}$$

where $\hat{A}_{\mathrm{H}}(\mathbf{x}, t)$ could be $\hat{\phi}_{\mathrm{H}}(\mathbf{x}, t)$, $\hat{\pi}_{\mathrm{H}}(\mathbf{x}, t)$ or a function of both, and $\chi = \varphi(\mathbf{x})$ or $\chi =$

$\pi(\mathbf{x})$. Note that $\hat{A}_{\mathtt{H}}(\mathbf{x},0) = \hat{A}_{\mathtt{S}}(\mathbf{x})$ and $|\chi\,;0\rangle_{\mathtt{H}} = |\chi\rangle_{\mathtt{S}}$. Here, the subscript H signifies the Heisenberg picture. In Dirac picture, also called the Interaction picture, quantum states, operators and basis vectors all evolve with time. The quantum states in this picture are defined by:

$$|\Psi;t\rangle_{\mathtt{I}} = \mathrm{e}^{iH_{\mathtt{S}}t}\,|\Psi;t\rangle_{\mathtt{S}}\,, \tag{5.104}$$

and the operators $\hat{A}_{\mathtt{I}}(\mathbf{x},t)$ are identified via the relation:

$$_{\mathtt{I}}\langle\,\Psi;t|\hat{A}_{\mathtt{I}}(\mathbf{x},t)|\Psi;t\rangle_{\mathtt{I}} = {}_{\mathtt{S}}\langle\,\Psi;t|\hat{A}_{\mathtt{S}}(\mathbf{x})\,|\Psi;t\rangle_{\mathtt{S}}\,, \tag{5.105}$$

which leads to:

$$\hat{A}_{\mathtt{I}}(\mathbf{x},t) = \mathrm{e}^{iH_{\mathtt{S}}t}\,\hat{A}_{\mathtt{S}}(\mathbf{x})\,\mathrm{e}^{-iH_{\mathtt{S}}t}\,. \tag{5.106}$$

Employing (5.104) in the Schrödinger equation, $i\,\partial_t|\Psi;t\rangle_{\mathtt{S}} = (H_{\mathtt{S}} + V_{\mathtt{S}})|\Psi;t\rangle_{\mathtt{S}}$, we obtain the equation governing the ket-states in the interaction picture:

$$i\,\partial_t|\Psi;t\rangle_{\mathtt{I}} = V_{\mathtt{I}}(t)|\Psi;t\rangle_{\mathtt{I}}\,, \qquad V_{\mathtt{I}}(t) = \mathrm{e}^{iH_{\mathtt{S}}t}\,V_{\mathtt{S}}\,\mathrm{e}^{-iH_{\mathtt{S}}t}\,, \tag{5.107}$$

where $V_{\mathtt{I}}(t) = \int_{\mathbb{R}^3} d^3\mathbf{x}\,\mathcal{V}(\hat{\phi}_{\mathtt{I}}(\mathbf{x},t),\hat{\pi}_{\mathtt{I}}(\mathbf{x},t))$. A formal solution for (5.107) is:

$$|\Psi;t\rangle_{\mathtt{I}} = U_{\mathtt{I}}(t,t_0)|\Psi;t_0\rangle_{\mathtt{I}}\,, \qquad U_{\mathtt{I}}(t,t_0) = \mathbf{T}\left\{\mathrm{e}^{-i\int_{t_0}^{t}dt'\,V_{\mathtt{I}}(t')}\right\}, \tag{5.108}$$

where $\mathbf{T}$ denotes the time ordering product. From (5.104) and (5.108), we deduce the following identities:

$$U_{\mathtt{S}}(t,t_0) = \mathrm{e}^{-iH_{\mathtt{S}}t}\,U_{\mathtt{I}}(t,t_0)\,\mathrm{e}^{iH_{\mathtt{S}}t_0}\,, \qquad U_{\mathtt{I}}(t,t_0) = \mathrm{e}^{iH_{\mathtt{S}}t}\,U_{\mathtt{S}}(t,t_0)\,\mathrm{e}^{-iH_{\mathtt{S}}t_0}\,, \tag{5.109}$$

where $U_{\mathtt{S}}(t,t_0)$ is the Schrödinger time evolution operator:

$$U_{\mathtt{S}}(t,t_0) = \mathrm{e}^{-i(H_{\mathtt{S}}+V_{\mathtt{S}})(t-t_0)}\,. \tag{5.110}$$

In the interaction picture the basis eigenkets $|\chi\,;t\rangle_{\mathtt{I}}$ evolve with time according to:

$$|\chi\,;t\rangle_{\mathtt{I}} = \mathrm{e}^{iH_{\mathtt{S}}t}\,|\chi\rangle_{\mathtt{S}}\,. \tag{5.111}$$

The path integral representation for the matrix element ${}_{\rm I}\langle\,\phi_b\,;t_b|\,U_{\rm I}(t_b,t_a)|\phi_a\,;t_a\rangle_{\rm I}$ is given by:

$$
\begin{aligned}
{}_{\rm I}\langle\,\phi_b\,;t_b|\,U_{\rm I}(t_b,t_a)|\phi_a\,;t_a\rangle_{\rm I} &= {}_{\rm S}\langle\,\phi_b|\,U_{\rm S}(t_b,t_a)|\phi_a\rangle_{\rm S} = {}_{\rm H}\langle\,\phi_b;t_b|\,|\phi_a;t_a\rangle_{\rm H} \\
&= \int_{\phi_a}^{\phi_b}\mathcal{D}\phi\int\mathcal{D}'\pi\,\exp\left(i\int_{t_a}^{t_b}dt\int_{\mathbb{R}^3}d^3\mathbf{x}\,\left[\pi(\mathbf{x},t)\dot{\phi}(\mathbf{x},t)-\mathcal{H}-\mathcal{V}\right]\right), \qquad (5.112)
\end{aligned}
$$

where $\mathcal{H}=\mathcal{H}(\phi(\mathbf{x},t),\pi(\mathbf{x},t))$ and $\mathcal{V}=\mathcal{V}(\phi(\mathbf{x},t),\pi(\mathbf{x},t))$. Here, unlike $\pi(\mathbf{x},t)$, the scalar fields $\phi(\mathbf{x},t)$ over which we integrate are constrained to the specific configurations $\phi_a(\mathbf{x})$ and $\phi_b(\mathbf{x})$ at times t_a and t_b respectively.

Now, we shall return to (5.101) to show how it can be expressed as a functional integral with the propagator arguments $\varphi(\mathbf{x})$ and $\varphi_0(\mathbf{x})$ acting as source fields rather than boundary conditions. Starting from (5.106), we deduce that:

$$
\mathrm{e}^{itH}\hat{\pi}(\mathbf{x}_1)\,\hat{\pi}(\mathbf{x}_2)\ldots\hat{\pi}(\mathbf{x}_n)=\hat{\pi}_{\rm I}(\mathbf{x}_1,t)\hat{\pi}_{\rm I}(\mathbf{x}_2,t)\ldots\hat{\pi}_{\rm I}(\mathbf{x}_n,t)\,\mathrm{e}^{itH}\,, \qquad (5.113)
$$

from which we can show that:

$$
\mathrm{e}^{-iTH}\;\mathrm{e}^{-i\int dx\,\varphi_0(\mathbf{x})\,\hat{\pi}(\mathbf{x})}=\mathrm{e}^{-i\int dx\,\varphi_0(\mathbf{x})\,\hat{\pi}_{\rm I}(\mathbf{x},-T)}\;\mathrm{e}^{-iTH}\,, \qquad (5.114)
$$

where H and $\hat{\pi}$ stand for the Schrödinger picture operators $H_{\rm S}$ and $\hat{\pi}_{\rm S}$ defined, respectively, in (5.102). By substituting (5.114) into (5.101) and making use of the fact that:

$$
\mathrm{e}^{i\int dx\,\varphi(\mathbf{x})\,\hat{\pi}(\mathbf{x})}\;\mathrm{e}^{-i\int dx\,\varphi_0(\mathbf{x})\,\hat{\pi}_{\rm I}(\mathbf{x},-T)}=\mathbf{T}\left\{\mathrm{e}^{i\int dx\,[\,\varphi(\mathbf{x})\hat{\pi}_{\rm I}(\mathbf{x},0)-\varphi_0(\mathbf{x})\hat{\pi}_{\rm I}(\mathbf{x},-T)\,]}\right\}, \qquad (5.115)
$$

for $T>0$, we arrive at:

$$
K[\varphi,\varphi_0;T]={}_{\rm I}\langle\varphi_{\rm D}\,;0|\,\mathbf{T}\left\{\mathrm{e}^{i\int dx\,[\,\varphi(\mathbf{x})\hat{\pi}_{\rm I}(\mathbf{x},0)-\varphi_0(\mathbf{x})\hat{\pi}_{\rm I}(\mathbf{x},-T)\,]}\right\}|\varphi_{\rm D}\,;-T\rangle_{\rm I}\,. \qquad (5.116)
$$

To simplify this expression further, we introduce the function:

$$
J(\mathbf{x},t)=2\,\varphi(\mathbf{x})\,\delta(t)-2\,\varphi_0(\mathbf{x})\,\delta(t+T)\,, \qquad (5.117)
$$

such that:

$$\int_{-T}^{0} dt \int d\mathbf{x}\, J(\mathbf{x},t)\,\hat{\pi}_{\mathrm{I}}(\mathbf{x},t) = \int d\mathbf{x}\,[\,\varphi(\mathbf{x})\hat{\pi}_{\mathrm{I}}(\mathbf{x},0) - \varphi_0(\mathbf{x})\hat{\pi}_{\mathrm{I}}(\mathbf{x},-T)\,]\,, \tag{5.118}$$

where we have adopted as a definition for the Dirac δ-function:

$$\delta(t) = \lim_{\epsilon\to 0}\delta_\epsilon(t)\,, \qquad \delta_\epsilon(t) = \begin{cases} \dfrac{1}{2\,\epsilon} & \text{for } |t| \le \epsilon \\ 0 & \text{for } |t| > \epsilon\,. \end{cases} \tag{5.119}$$

Now, we can rewrite (5.116) in a form:

$$K[\varphi,\varphi_0;T] = {}_{\mathrm{I}}\langle\varphi_{\mathrm{D}}\,;0|\,\mathbf{T}\left\{\mathrm{e}^{i\int_{-T}^{0} dt\int d\mathbf{x}\, J(\mathbf{x},t)\hat{\pi}_{\mathrm{I}}(\mathbf{x},t)}\right\}|\varphi_{\mathrm{D}}\,;-T\rangle_{\mathrm{I}}\,, \tag{5.120}$$

which allows for the path integral representation as illustrated in (5.112), giving:

$$K[\varphi,\varphi_0;T] = \int_{\phi=0}^{\phi=0}\mathcal{D}\phi\int\mathcal{D}'\pi\ \exp\left(i\int_{-T}^{0}dt\int_{\mathbb{R}^3}d^3\mathbf{x}\,\left[\pi(\mathbf{x},t)\,\xi(\mathbf{x},t) - \mathcal{H}\right]\right), \tag{5.121}$$

where $\xi(\mathbf{x},t) = \dot{\phi}(\mathbf{x},t) + J(\mathbf{x},t)$. For quadratic Hamiltonians in $\pi(\mathbf{x},t)$:

$$H = \int_{\mathbb{R}^3} d^3\mathbf{x}\,\mathcal{H}(\phi,\pi) = \int_{\mathbb{R}^3} d^3\mathbf{x}\,\Big[\mathcal{H}_0(\phi,\pi) + g\,\mathcal{H}_1(\phi)\Big]\,, \qquad g \ge 0\,, \tag{5.122}$$

where $\mathcal{H}_0(\phi,\pi)$ is given by (5.3) and $\mathcal{H}_1(\phi)$ is a polynomial in $\phi(\mathbf{x},t)$, we can easily evaluate the π-integral in (5.121) to obtain:

$$K[\varphi,\varphi_0;T] = C\int_{\phi=0}^{\phi=0}\mathcal{D}\phi\ \exp\left(i\int_{-T}^{0}dt\int_{\mathbb{R}^3}d^3\mathbf{x}\,\left[\,\mathcal{L}(\phi,\dot{\phi}) + \dot{\phi}\,J + \frac{1}{2}\,J^2\,\right]\right), \tag{5.123}$$

where $\mathcal{L} = \mathcal{L}_0(\phi,\dot{\phi}) - g\,\mathcal{H}_1(\phi)$ with $\mathcal{L}_0$ given by (5.1), and C is a constant equal to $\int\mathcal{D}'\eta\ \exp\Big(-i\int_{-T}^{0}dt\int_{\mathbb{R}^3}d^3\mathbf{x}\ \eta^2(\mathbf{x},t)/2\Big)$. Substituting (5.117) into (5.123) gives:

$$K[\varphi,\varphi_0;T] = C\int_{\phi=0}^{\phi=0}\mathcal{D}\phi\ \exp\Big(iS[\phi] + i\mathcal{J}[\varphi,\varphi_0\,;\phi]\Big)\,, \tag{5.124}$$

where

$$S[\phi] = \int_{-T}^{0} dt \int_{\mathbb{R}^3} d^3\mathbf{x}\, \mathcal{L}(\phi, \dot{\phi}) = \int_{-T}^{0} dt \int_{\mathbb{R}^3} d^3\mathbf{x}\, \Big[\mathcal{L}_0(\phi, \dot{\phi}) - g\, \mathcal{H}_1(\phi)\Big], \tag{5.125}$$

$$\mathcal{J}[\varphi, \varphi_0\,; \phi] = \int_{\mathbb{R}^3} d^3\mathbf{x}\, \Big[\varphi(\mathbf{x})\, \dot{\phi}(\mathbf{x}, 0) - \varphi_0(\mathbf{x})\, \dot{\phi}(\mathbf{x}, -T) + \delta(0)\, (\varphi^2 + \varphi_0^2)\Big]. \tag{5.126}$$

Here, we remark that the boundary condition on the integration variable ϕ is that it should vanish on the boundary surfaces at $t = 0$ and $t = -T$ as implied in (5.116) by φ_{D}, on the other hand the arguments of the propagation kernel φ and φ_0 act as source fields on the boundary surfaces $t = 0$ and $t = -T$, respectively. Now, by using (5.124) in (5.96) we obtain the path integral representation for the Schrödinger vacuum functional $\Psi_0[\varphi]$,

$$\Psi_0[\varphi] = \lim_{T \to -i\infty} \frac{\int_{\phi=0}^{\phi=0} \mathcal{D}\phi\, \exp\Big(iS[\phi] + i\int_{\mathbb{R}^3} d^3\mathbf{x} \Big[\varphi(\mathbf{x})\, \dot{\phi}(\mathbf{x}, 0) + \delta(0)\varphi^2(\mathbf{x})\Big]\Big)}{\int_{\phi=0}^{\phi=0} \mathcal{D}\phi\, \exp\Big(iS[\phi]\Big)}, \tag{5.127}$$

with the field eigenvalue $\varphi(\mathbf{x})$ acting as a source field on the boundary surface $t = 0$. Here, the linearly divergent term in the exponent, namely $\delta(0) \int_{\mathbb{R}^3} d^3\mathbf{x}\, \varphi^2(\mathbf{x})$, plays the role of a counter term which is required to cancel a singular contribution that arises from the surface term $\int_{\mathbb{R}^3} d^3\mathbf{x}\, \varphi(\mathbf{x})\, \dot{\phi}(\mathbf{x}, 0)$ as we try to integrate (5.127) over the fields $\phi(\mathbf{x}, t)$. We shall show this in the next section.

5.5 The Vacuum in Perturbation Field Theory

In this section, we shall illustrate one of the perturbative methods that can be used in the Schrödinger representation to approximate the vacuum functional $\Psi_0[\varphi]$ for a self-interacting scalar field. In particular, we shall calculate the unrenormalised form of the vacuum functional for ϕ^4-theory to one-loop order. We shall also check our results with the free theory case.

Throughout this section, we shall work in Euclidean space-time in which the vacuum functional (5.127) assumes the form:

$$\Psi_0[\varphi] = N(g) \int_{\phi=0}^{\phi=0} \mathcal{D}\phi\, \exp\Big(-\, S_E[\phi] - \int_{\partial\Gamma} d^3\mathbf{x}\, \Big[\varphi(\mathbf{x})\, \dot{\phi}(\mathbf{x}, 0) + \delta(0)\, \varphi^2(\mathbf{x})\Big]\Big), \tag{5.128}$$

where $1/N(g) = \int_{\phi=0}^{\phi=0} \mathcal{D}\phi \, \exp\Big(- S_E[\phi]\Big)$, and the Euclidean action $S_E[\phi]$ is given by:

$$S_E[\phi] = S_E^{(0)}[\phi] + g \int_\Gamma d^4x \, \mathcal{H}_1(\phi)\,, \qquad S_E^{(0)}[\phi] = \int_\Gamma d^4x \;\; \mathcal{L}_E^{(0)}(\phi, \dot\phi)\,, \tag{5.129}$$

$$\mathcal{L}_E^{(0)}(\phi, \dot\phi) = \frac{1}{2}\Big[(\partial_\mu\phi)^2 + m^2\phi^2\Big] = \frac{1}{2}\Big[\dot\phi^2 + (\nabla\phi)^2 + m^2\phi^2\Big]\,. \tag{5.130}$$

Here, we denote by Γ the Euclidean half space-time region defined by the set of points $\{(\mathbf{x}, t) : \mathbf{x} \in \mathbb{R}^3,\ t \leq 0\}$, and use $\partial\Gamma$ to designate the $t = 0$ boundary surface $\{(\mathbf{x}, t) : \mathbf{x} \in \mathbb{R}^3,\ t = 0\}$. Note that in continuing to Euclidean space-time, the Minkowski δ-function $\delta(t)$ is replaced by $i\delta(t)$, see Ref. [61].

To compute the functional integral in (5.128), we introduce an auxiliary functional of $\varphi(\mathbf{x})$ and $\rho(\mathbf{x}, t)$:

$$\Psi_0[\varphi, \rho] = N(g) \int_{\phi=0}^{\phi=0} \mathcal{D}\phi \;\; \exp\Big(- S_E[\phi] + \mathcal{K}[\phi, \varphi, \rho] - \delta(0) \int_{\partial\Gamma} d^3\mathbf{x} \, \varphi^2(\mathbf{x})\Big), \tag{5.131}$$

such that $\Psi_0[\varphi, 0] = \Psi_0[\varphi]$, where ρ is an additional source field coupled to ϕ in:

$$\mathcal{K}[\phi, \varphi, \rho] = \int_\Gamma d^4x \, \Big[\phi(x)\,\rho(x) - 2\,\delta(t)\,\varphi(\mathbf{x})\,\dot\phi(x)\Big] = \int_\Gamma d^4x \;\phi(x)\,\sigma(x)\,, \tag{5.132}$$

with
$$\sigma(x) = \rho(x) + 2\,\dot\delta(t)\,\varphi(\mathbf{x})\,, \qquad \dot\delta(t) = \frac{d}{dt}\,\delta(t)\,, \qquad x = (\mathbf{x}, t)\,. \tag{5.133}$$

In what follows, we shall mainly consider $\Psi_0[\varphi, \rho]$ because it reduces to $\Psi_0[\varphi]$ when $\rho(x) = 0$. By making use of the following identity:

$$\mathcal{H}_1\left(\frac{\delta}{\delta\rho(x)}\right) \exp\Big(\int_\Gamma d^4y \, \phi(y)\,\rho(y)\Big) = \mathcal{H}_1(\phi(x)) \;\exp\Big(\int_\Gamma d^4y \, \phi(y)\,\rho(y)\Big), \tag{5.134}$$

we can rewrite (5.131) as:

$$\Psi_0[\varphi, \rho] = \overline{N}(g) \;\exp\left(- g \int_\Gamma d^4x \, \mathcal{H}_1\left(\frac{\delta}{\delta\rho(x)}\right)\right) \Psi_0^{(0)}[\varphi, \rho]\,, \tag{5.135}$$

where $\overline{N}(g) = N(g)/N(0)$, and $\Psi_0^{(0)}[\varphi, \rho] = \Psi_0[\varphi, \rho]\Big|_{g=0}$ assumes the form:

$$\Psi_0^{(0)}[\varphi, \rho] = N(0) \int_{\phi=0}^{\phi=0} \mathcal{D}\phi \;\exp\Big(- S_E^{(0)}[\phi] + \mathcal{K}[\phi, \varphi, \rho] - \delta(0) \int_{\partial\Gamma} d^3\mathbf{x} \, \varphi^2(\mathbf{x})\Big). \tag{5.136}$$

Note that since $1/N(0) = \int_{\phi=0}^{\phi=0} \mathcal{D}\phi \, \exp\Big(-S_E^{(0)}[\phi]\Big)$, we have $\Psi_0^{(0)}[0,0] = 1$.

Let us now evaluate the functional integral representing $\Psi_0^{(0)}[\varphi,\rho]$ in (5.136), illustrating the removal of the divergent term $\delta(0)\int_{\mathbb{R}^3} d^3\mathbf{x}\ \varphi^2(\mathbf{x})$. Consider changing the integration variables in (5.136) as:

$$\phi(x) \to \bar{\phi}(x) = \phi(x) - \phi_c(x)\,, \qquad \mathcal{D}\phi = \mathcal{D}\bar{\phi}\,, \tag{5.137}$$

where $\phi_c(x)$ is a solution of the differential equation:

$$(-\partial^2 + m^2)\phi_c(x) = \sigma(x), \qquad \partial^2 = \frac{\partial^2}{\partial t^2} + \nabla^2\,, \tag{5.138}$$

satisfying the Dirichlet boundary conditions:

$$\phi_c(x)\big|_{t=0} = \phi_c(\mathbf{x},0) = 0\,, \qquad \phi_c(x)\big|_{t=-\infty} = \phi_c(\mathbf{x},-\infty) = 0\,. \tag{5.139}$$

Since both $\phi_c(x)$ and $\phi(x)$ satisfy the Dirichlet boundary conditions, so does $\bar{\phi}(x)$ as can be seen from (5.137). Using (5.137) in (5.136) together with the fact that:

$$S_E^{(0)}[\bar{\phi}+\phi_c] = S_E^{(0)}[\bar{\phi}] + S_E^{(0)}[\phi_c] + \int_\Gamma d^4x\ \bar{\phi}(x)\,\sigma(x)\,, \tag{5.140}$$

gives:

$$\Psi_0^{(0)}[\varphi,\rho] = \exp\Big(-S_E^{(0)}[\phi_c] + \int_\Gamma d^4x\ \phi_c(x)\,\sigma(x) - \delta(0)\int_{\partial\Gamma} d^3\mathbf{x}\ \varphi^2(\mathbf{x})\Big)\,, \tag{5.141}$$

which, after some manipulations, we can write as:

$$\Psi_0^{(0)}[\varphi,\rho] = \exp\Big(\frac{1}{2}\int_\Gamma d^4x\ \phi_c(x)\,\sigma(x) - \delta(0)\int_{\partial\Gamma} d^3\mathbf{x}\ \varphi^2(\mathbf{x})\Big)\,. \tag{5.142}$$

In Appendix B, we find $\phi_c(x)$ to be:

$$\phi_c(x) = \int_\Gamma d^4x'\ G_D(x;x')\,\sigma(x')\,, \tag{5.143}$$

where

$$G_D(x;x') = G_D(\mathbf{x}-\mathbf{x}';t,t') = \Delta_F(\mathbf{x}-\mathbf{x}';t-t') - \Delta_F(\mathbf{x}-\mathbf{x}';t+t')\,, \tag{5.144}$$

with $\Delta_F(\mathbf{y}\,;y_0)$ being the Feynman propagator in Euclidean space-time:

$$\Delta_F(\mathbf{y};y_0) = \int_{\mathbb{R}^4} \frac{d^4k}{(2\pi)^4}\ \frac{1}{k^2+m^2}\ \mathrm{e}^{ik_0y_0+i\mathbf{k}.\mathbf{y}}\,, \qquad k^2 = k_0^2+\mathbf{k}^2\,. \tag{5.145}$$

Taking $\sigma(x)$ as defined in (5.133) and substituting into (5.143), yields:

$$\phi_c(x) = \int_\Gamma d^4x'\ G_D(x;x')\,\rho(x') - \int_{\partial\Gamma} d^3\mathbf{x}'\ \varphi(\mathbf{x}')\,\partial_{t'}G_D(x;x')\big|_{t'=0}\,. \tag{5.146}$$

Using this together with (5.133) in (5.142) gives:

$$\Psi_0^{(0)}[\varphi,\rho] = \mathrm{e}^{\mathfrak{X}[\varphi,\rho]}\,, \tag{5.147}$$

where

$$\begin{aligned}\mathfrak{X}[\varphi,\rho] = \frac{1}{2}\int_\Gamma\int_\Gamma d^4x\,d^4x'\ \ &\rho(x)\,G_D(x;x')\,\rho(x')\\ &-\int_\Gamma\int_{\partial\Gamma} d^4x'\,d^3\mathbf{x}\ \ \rho(x')\,\varphi(\mathbf{x})\ \partial_t G_D(x;x')\big|_{t=0}\\ &+\frac{1}{2}\int_{\partial\Gamma}\int_{\partial\Gamma} d^3\mathbf{x}\,d^3\mathbf{x}'\ \varphi(\mathbf{x})\,\varphi(\mathbf{x}')\ \partial_t\partial_{t'}G_D(x;x')\big|_{t=t'=0}\\ &-\delta(0)\int_{\partial\Gamma} d^3\mathbf{x}\ \varphi^2(\mathbf{x})\,.\end{aligned} \tag{5.148}$$

To show how the last term in (5.148) is removed, we calculate $\partial_t\partial_{t'}G_D(x;x')$ for $t=t'=0$, giving:

$$\begin{aligned}\partial_t\partial_{t'}G_D(x;x')\big|_{t=t'=0} &= 2\int_{\mathbb{R}^4}\frac{d^4k}{(2\pi)^4}\ \frac{k_0^2}{k^2+m^2}\ \mathrm{e}^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}')}\\ &= 2\int_{\mathbb{R}^4}\frac{d^4k}{(2\pi)^4}\left[1-\frac{\mathbf{k}^2+m^2}{k_0^2+\mathbf{k}^2+m^2}\right]\mathrm{e}^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}')}\\ &= 2\,\delta(0)\ \delta(\mathbf{x}-\mathbf{x}') - (-\nabla^2+m^2)^{1/2}\,\delta(\mathbf{x}-\mathbf{x}')\,.\end{aligned} \tag{5.149}$$

Then by substituting this into the third term in (5.148), we eliminate the singular contri-

bution of $\delta(0)$, obtaining:

$$\begin{aligned}\mathfrak{X}[\varphi,\rho] = &\frac{1}{2}\int_\Gamma\int_\Gamma d^4x\, d^4x'\ \ \rho(x)\, G_D(x;x')\,\rho(x') \\ &- \int_\Gamma\int_{\partial\Gamma} d^4x'\, d^3\mathbf{x}\ \ \rho(x')\,\varphi(\mathbf{x})\ \partial_t G_D(x;x')\big|_{t=0} \\ &- \frac{1}{2}\int_{\partial\Gamma} d^3\mathbf{x}\ \varphi(\mathbf{x})\,(-\nabla^2+m^2)^{1/2}\,\varphi(\mathbf{x})\,. \end{aligned} \tag{5.150}$$

Using this and (5.147) in (5.135) gives:

$$\Psi_0[\varphi,\rho] = \exp\left(-\frac{1}{2}\int_{\partial\Gamma} d^3\mathbf{x}\ \varphi(\mathbf{x})\,(-\nabla^2+m^2)^{1/2}\,\varphi(\mathbf{x})\right) Z[\varphi,\rho]\,, \tag{5.151}$$

where

$$Z[\varphi,\rho] = \overline{N}(g)\ \exp\left(-g\int_\Gamma d^4x\ \mathcal{H}_1\left(\frac{\delta}{\delta\rho(x)}\right)\right)\ Z_0[\varphi,\rho]\,, \tag{5.152}$$

with $Z_0[\varphi,\rho] = \exp\big(W_0[\varphi,\rho]\big)$, and

$$\begin{aligned}W_0[\varphi,\rho] = &\frac{1}{2}\int_\Gamma\int_\Gamma d^4x\, d^4x'\ \ \rho(x)\, G_D(x;x')\,\rho(x') \\ &- \int_\Gamma\int_{\partial\Gamma} d^4x'\, d^3\mathbf{x}\ \ \rho(x')\,\varphi(\mathbf{x})\ \partial_t G_D(x;x')\big|_{t=0}\,. \end{aligned} \tag{5.153}$$

Now, the Schrödinger vacuum functional for a self-interacting scalar field is obtained from (5.151) by simply setting $\rho(x)$ to zero, i.e. $\Psi_0[\varphi,0] = \Psi_0[\varphi]$. For $g=0$, $\Psi_0[\varphi,0]$ reduces to the free vacuum functional obtained earlier in (5.67), but with a normalisation constant $\mathcal{N}=1$ to meet with our choice $\Psi_0[0]=1$.

The new form of $\Psi_0[\varphi,\rho]$, given by (5.151), saves us from the problem of evaluating the functional integral (5.131) of the full interacting theory, which we could not have achieved anyway since we know only how to do Gaussian integrals. As compensation, expression (5.151) contains a complicated combination of functional derivatives. However, it still allows for the standard perturbative expansion which provides good approximation for small values of g, i.e. in the case of weak interactions. Now, we shall illustrate the perturbative calculation of (5.151). We begin by expanding the exponential $\exp\left(-g\int_\Gamma d^4x\ \mathcal{H}_1\left(\frac{\delta}{\delta\rho(x)}\right)\right)$ in (5.152), and writing:

$$Z[\varphi,\rho] = \overline{N}(g)\, Z_0[\varphi,\rho]\left(1 + g\,\mathcal{U}_1[\varphi,\rho] + g^2\,\mathcal{U}_2[\varphi,\rho] + g^3\,\mathcal{U}_3[\varphi,\rho]\ldots\right), \tag{5.154}$$

where

$$\mathcal{U}_n[\varphi,\rho] = \frac{(-1)^n}{n!}\left(Z_0[\varphi,\rho]\right)^{-1}\Big[\prod_{i=1}^{n}\int_\Gamma d^4x_i\,\mathcal{H}_1\left(\frac{\delta}{\delta\rho(x_i)}\right)\Big]Z_0[\varphi,\rho]\,. \tag{5.155}$$

Note that the normalization factor $\overline{N}(g)$, which is independent of both φ and ρ, assumes the form:

$$\overline{N}(g) = \frac{\int_{\phi=0}^{\phi=0}\mathcal{D}\phi\,\exp\left(-S_E^{(0)}[\phi]\right)}{\int_{\phi=0}^{\phi=0}\mathcal{D}\phi\,\exp\left(-S_E[\phi]\right)}\,, \tag{5.156}$$

which can be rewritten as:

$$\begin{aligned}\overline{N}(g) &= \left[\exp\left(-g\int_\Gamma d^4x\,\mathcal{H}_1\left(\frac{\delta}{\delta\rho(x)}\right)\right)Z_0[0,\rho]\Big|_{\rho=0}\right]^{-1}\\ &= \left(1+g\,\mathcal{U}_1[0,0]+g^2\,\mathcal{U}_2[0,0]+g^3\,\mathcal{U}_3[0,0]\ldots\right)^{-1}.\end{aligned} \tag{5.157}$$

Substituting this in (5.154) yields:

$$Z[\varphi,\rho] = Z_0[\varphi,\rho]\;\frac{1+g\,\mathcal{U}_1[\varphi,\rho]+g^2\,\mathcal{U}_2[\varphi,\rho]+g^3\,\mathcal{U}_3[\varphi,\rho]\ldots}{1+g\,\mathcal{U}_1[0,0]+g^2\,\mathcal{U}_2[0,0]+g^3\,\mathcal{U}_3[0,0]\ldots}\,. \tag{5.158}$$

To obtain a power series representation in g, we compute the division of the two series in (5.158), using the following formula [51]:

$$\frac{\sum_{n=0}^{\infty}a_n\,x^n}{\sum_{n=0}^{\infty}b_n\,x^n} = \sum_{n=1}^{\infty}c_n\,x^n, \qquad c_n = (-1)^n\begin{vmatrix} b_1-a_1 & 1 & 0 & \cdots & 0\\ b_2-a_2 & b_1 & 1 & \cdots & 0\\ b_3-a_3 & b_2 & b_1 & \cdots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ b_n-a_n & b_{n-1} & b_{n-2} & \cdots & b_1\end{vmatrix}, \tag{5.159}$$

with $a_0 = 1$, $b_0 = 1$ and $c_0 = 1$. This allows us to rewrite (5.158) as:

$$Z[\varphi,\rho] = Z_0[\varphi,\rho]\left(1+g\,\mathcal{Z}_1[\varphi,\rho]+g^2\,\mathcal{Z}_2[\varphi,\rho]+g^3\,\mathcal{Z}_3[\varphi,\rho]+\ldots\right), \tag{5.160}$$

where

$$\mathcal{Z}_1[\varphi,\rho] = \mathcal{U}_1[\varphi,\rho] - \mathcal{U}_1[0,0]\,, \tag{5.161}$$

$$\mathcal{Z}_2[\varphi,\rho] = \mathcal{U}_2[\varphi,\rho] - \mathcal{U}_2[0,0] - \Big(\mathcal{U}_1[\varphi,\rho] - \mathcal{U}_1[0,0]\Big)\,\mathcal{U}_1[0,0]\,, \tag{5.162}$$

$$\begin{aligned}\mathcal{Z}_3[\varphi,\rho] = {} & \mathcal{U}_3[\varphi,\rho] - \mathcal{U}_3[0,0] - \Big(\mathcal{U}_2[\varphi,\rho] - \mathcal{U}_2[0,0]\Big)\,\mathcal{U}_1[0,0] \\ & + \Big(\mathcal{U}_1[\varphi,\rho] - \mathcal{U}_1[0,0]\Big)\Big(\mathcal{U}_1^2[0,0] - \mathcal{U}_2[0,0]\Big)\,, \qquad \textit{etc.}\end{aligned} \tag{5.163}$$

We note that all terms contain factors of the type $\big(\mathcal{U}_n[\varphi,\rho]-\mathcal{U}_n[0,0]\big)$. This clearly implies $\mathcal{Z}_n[0,0] = 0$, thus ensuring that our choice of the normalization condition $\Psi_0[0,0] = 1$ is met since in (5.151) $Z[0,0] = 1$.

For illustration, we shall now consider the ϕ^4-theory to one-loop order. The Euclidean Lagrangian density for this model is given by:

$$\mathcal{L}_E = \frac{1}{2}\left(\dot{\phi}^2 + (\nabla\phi)^2 + m^2\,\phi^2\right) + g\,\mathcal{H}_1(\phi)\,, \tag{5.164}$$

with the interaction term:

$$g\,\mathcal{H}_1(\phi) = \frac{g}{4!}\,\phi^4(x)\,. \tag{5.165}$$

The corresponding Schrödinger vacuum functional for this model follows from (5.151) as:

$$\Psi_0[\varphi] = \Psi_0[\varphi,0] = \exp\left(-\frac{1}{2}\int_{\partial\Gamma} d^3\mathbf{x}\;\varphi(\mathbf{x})\,(-\nabla^2 + m^2)^{1/2}\,\varphi(\mathbf{x})\right) Z[\varphi,0]\,. \tag{5.166}$$

In perturbation theory to one-loop order, (5.160) gives:

$$Z[\varphi,0] = 1 + g\;\mathcal{Z}_1[\varphi,0] + O(g^2)\,, \tag{5.167}$$

where

$$\mathcal{Z}_1[\varphi,0] = \mathcal{U}_1[\varphi,0] - \mathcal{U}_1[0,0] = -\frac{1}{4!}\int_\Gamma d^4x\left[\frac{\delta^4 Z_0[\varphi,\rho]}{\delta\rho^4(x)}\bigg|_{\rho=0} - \frac{\delta^4 Z_0[0,\rho]}{\delta\rho^4(x)}\bigg|_{\rho=0}\right]. \tag{5.168}$$

Note that $Z_0[\varphi,0] = \exp(W_0[\varphi,0]) = 1$. The $4th$ functional derivative of $Z_0[\varphi,\rho]$ with

respect to ρ is:

$$\frac{\delta^4 Z_0[\varphi,\rho]}{\delta\rho^4(x)} = Z_0[\varphi,\rho]\left[\frac{\delta^4 W_0[\varphi,\rho]}{\delta\rho^4(x)} + 4\,\frac{\delta W_0[\varphi,\rho]}{\delta\rho(x)}\,\frac{\delta^3 W_0[\varphi,\rho]}{\delta\rho^3(x)} + 3\left(\frac{\delta^2 W_0[\varphi,\rho]}{\delta\rho^2(x)}\right)^2 + 6\left(\frac{\delta W_0[\varphi,\rho]}{\delta\rho(x)}\right)^2\frac{\delta^2 W_0[\varphi,\rho]}{\delta\rho^2(x)} + \left(\frac{\delta W_0[\varphi,\rho]}{\delta\rho(x)}\right)^4\right], \tag{5.169}$$

where

$$\frac{\delta W_0[\varphi,\rho]}{\delta\rho(x)} = \int_\Gamma d^4x'\;\rho(x')\;G_D(x;x') - \int_{\partial\Gamma} d^3\mathbf{x}'\;\;\varphi(\mathbf{x}')\,\partial_{t'}G_D(x;x')\big|_{t'=0}, \tag{5.170}$$

$$\frac{\delta^2 W_0[\varphi,\rho]}{\delta\rho^2(x)} = G_D(x;x), \tag{5.171}$$

$$\frac{\delta^3 W_0[\varphi,\rho]}{\delta\rho^3(x)} = \frac{\delta^4 W_0[\varphi,\rho]}{\delta\rho^4(x)} = 0. \tag{5.172}$$

This gives:

$$\left.\frac{\delta^4 Z_0[\varphi,\rho]}{\delta\rho^4(x)}\right|_{\rho=0} = 3\;G_D^2(x;x) + 6\;G_D(x;x)\prod_{j=1}^{2}\int_{\partial\Gamma} d^3\mathbf{x}_j\;\;\varphi(\mathbf{x}_j)\,\partial_{t_j}G_D(x_j;x)\big|_{t_j=0} + \prod_{j=1}^{4}\int_{\partial\Gamma} d^3\mathbf{x}_j\;\;\varphi(\mathbf{x}_j)\,\partial_{t_j}G_D(x_j;x)\big|_{t_j=0}, \tag{5.173}$$

$$\left.\frac{\delta^4 Z_0[0,\rho]}{\delta\rho^4(x)}\right|_{\rho=0} = 3\;G_D^2(x;x), \tag{5.174}$$

where $G_D(x;x)$ and $\partial_{t_j}G_D(x_j;x)\big|_{t_j=0}$ are calculated to be:

$$G_D(x;x) = \frac{1}{2}\int_{\mathbb{R}^3}\frac{d^3\mathbf{k}}{(2\pi)^3}\;\;\frac{1}{\sqrt{\mathbf{k}^2+m^2}}\left[1-\mathrm{e}^{2t\sqrt{\mathbf{k}^2+m^2}}\right], \tag{5.175}$$

$$\partial_{t_j}G_D(x_j;x)\big|_{t_j=0} = -\int_{\mathbb{R}^3}\frac{d^3\mathbf{k}}{(2\pi)^3}\;\;\mathrm{e}^{t\sqrt{\mathbf{k}^2+m^2}}\;\;\mathrm{e}^{i\mathbf{k}.(\mathbf{x}_j-\mathbf{x})}, \tag{5.176}$$

for $t < 0$, and zero for $t = 0$. Here, $G_D(x;x)$ is divergent. To see this, let us evaluate (5.175) using the spherical coordinates $\mathbf{k} = (p,\theta,\phi)$ with a cut off $p_{\max}$ imposed at a large

magnitude of $\mathbf{k}$. In this way, we can write:

$$\begin{aligned} G_D(x;x) &= \int_0^{p_{\max}} \frac{dp}{(2\pi)^2} \frac{p^2}{\sqrt{p^2+m^2}} \left[1 - \mathrm{e}^{2t\sqrt{p^2+m^2}}\right] \\ &= \frac{1}{2\,(2\pi)^2}\left[p_{\max}\sqrt{p_{\max}^2+m^2} + m^2 \ln\left(\frac{m}{p_{\max}+\sqrt{p_{\max}^2+m^2}}\right)\right] \\ &\quad - \int_0^{p_{\max}} \frac{dp}{(2\pi)^2} \frac{p^2}{\sqrt{p^2+m^2}} \mathrm{e}^{2t\sqrt{p^2+m^2}}. \end{aligned} \tag{5.177}$$

In the limit as $p_{\max} \to \infty$ the first term in (5.177) diverges while the second term tends to $m\,K_1(-2\,m\,t)/8\pi^2 t$, where $K_1(\xi \in \mathbb{R}^+)$ is the modified Bessel function. This is a problem regularly encountered in quantum field theory and is usually remedied by a renormalization procedure, see refs. [56,57] for more details.

Substituting (5.173) and (5.174) into (5.168) gives:

$$\begin{aligned} \mathcal{Z}_1[\varphi,0] &= \frac{1}{2!}\int_{\partial\Gamma} d^3\mathbf{x}_1\, d^3\mathbf{x}_2\ \mathfrak{J}_1^{(2)}(\mathbf{x}_1,\mathbf{x}_2)\,\varphi(\mathbf{x}_1)\,\varphi(\mathbf{x}_2) \\ &\quad + \frac{1}{4!}\int_{\partial\Gamma} d^3\mathbf{x}_1\, d^3\mathbf{x}_2\, d^3\mathbf{x}_3\, d^3\mathbf{x}_4\ \mathfrak{J}_1^{(4)}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4)\,\varphi(\mathbf{x}_1)\,\varphi(\mathbf{x}_2)\,\varphi(\mathbf{x}_3)\,\varphi(\mathbf{x}_4), \end{aligned} \tag{5.178}$$

where

$$\mathfrak{J}_1^{(2)}(\mathbf{x}_1,\mathbf{x}_2) = -\frac{1}{2}\int_\Gamma d^4x\ G_D(x;x) \prod_{j=1}^{2} \partial_{t_j} G_D(x_j;x)\big|_{t_j=0}, \tag{5.179}$$

$$\mathfrak{J}_1^{(4)}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3,\mathbf{x}_4) = -\int_\Gamma d^4x \prod_{j=1}^{4} \partial_{t_j} G_D(x_j;x)\big|_{t_j=0}. \tag{5.180}$$

In Euclidean momentum space, (5.178) assumes the form:

$$\begin{aligned} \mathcal{Z}_1[\widetilde{\varphi},0] &= \frac{1}{2!}\int_{\mathbb{R}^3} \frac{d^3\mathbf{k}_1}{(2\pi)^3}\frac{d^3\mathbf{k}_2}{(2\pi)^3}\ \widetilde{\mathfrak{J}}_1^{(2)}(\mathbf{k}_1,\mathbf{k}_2)\ \widetilde{\varphi}(\mathbf{k}_1)\,\widetilde{\varphi}(\mathbf{k}_2)\,(2\pi)^3\delta(\mathbf{k}_1+\mathbf{k}_2) \\ &\quad + \frac{1}{4!}\int_{\mathbb{R}^3} \frac{d^3\mathbf{k}_1}{(2\pi)^3}\cdots\frac{d^3\mathbf{k}_4}{(2\pi)^3}\,\widetilde{\mathfrak{J}}_1^{(4)}(\mathbf{k}_1,\ldots,\mathbf{k}_4)\,\widetilde{\varphi}(\mathbf{k}_1)\ldots\widetilde{\varphi}(\mathbf{k}_4)(2\pi)^3\delta(\mathbf{k}_1+\ldots+\mathbf{k}_4), \end{aligned} \tag{5.181}$$

where $\widetilde{\varphi}(\mathbf{k})$ is the Fourier transform inverse of $\varphi(\mathbf{x})$:

$$\varphi(\mathbf{x}) = \int_{\mathbb{R}^3} \frac{d^3\mathbf{k}}{(2\pi)^3}\ \widetilde{\varphi}(\mathbf{k})\,\mathrm{e}^{i\mathbf{k}.\mathbf{x}}, \qquad \widetilde{\varphi}(\mathbf{k}) = \int_{\mathbb{R}^3} d^3\mathbf{x}\ \varphi(\mathbf{x})\,\mathrm{e}^{-i\mathbf{k}.\mathbf{x}}, \tag{5.182}$$

and

$$\widetilde{\mathfrak{J}}_1^{(2)}(\mathbf{k}_1,\mathbf{k}_2) = -\frac{1}{4}\int_{\mathbb{R}^3}\frac{d^3\mathbf{p}}{(2\pi)^3}\,\frac{1}{\omega(\mathbf{p})}\left[\frac{1}{\omega(\mathbf{k_1})+\omega(\mathbf{k_2})} - \frac{1}{2\omega(\mathbf{p})+\omega(\mathbf{k_1})+\omega(\mathbf{k_2})}\right],$$

$$= -\frac{1}{8}\int_{\mathbb{R}^3}\frac{d^3\mathbf{p}}{(2\pi)^3}\,\frac{1}{\omega(\mathbf{k_1})}\,\frac{1}{\left[\omega(\mathbf{k_1})+\omega(\mathbf{p})\right]}\,, \qquad \mathbf{k_1}=-\mathbf{k_2}\,, \tag{5.183}$$

$$\widetilde{\mathfrak{J}}_1^{(4)}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4) = -\frac{1}{\omega(\mathbf{k_1})+\omega(\mathbf{k_2})+\omega(\mathbf{k_3})+\omega(\mathbf{k_4})}\,. \tag{5.184}$$

Here, $\omega(\mathbf{p})$ is defined in (5.7) as $\omega(\mathbf{p}) = \sqrt{\mathbf{p}^2+m^2}$. The logarithm of the vacuum functional $\mathsf{W}_0[\varphi] = \ln\Psi_0[\varphi,0]$ to one-loop order can now be written as:

$$\mathsf{W}_0[\varphi] = -\frac{1}{2}\int_{\partial\Gamma} d^3\mathbf{x}\;\varphi(\mathbf{x})\,(-\nabla^2+m^2)^{1/2}\,\varphi(\mathbf{x}) + g\,\mathcal{Z}_1[\varphi,0] + O(g^2)\,. \tag{5.185}$$

In general, the perturbative expansion of $\mathsf{W}_0[\varphi]$ is the actual sum of all the connected Feynman diagrams in which $\varphi(\mathbf{x})$ is the source field.

5.6 Analyticity and Local expansion of $\mathsf{W}_0[\varphi]$

In this section, we shall show that under a scale transformation of the source field $\varphi \to \varphi_s = \varphi(x/\sqrt{s})$ the logarithm of the resultant scaled vacuum functional, denoted by $\mathsf{W}_0[\varphi\,;s] = \mathsf{W}_0[\varphi_s]$, for a massive interacting scalar field theory in 1+1 dimensions is analytic in the cut complex s-plane with the branch cut on the negative real axis. This provides a novel approximation method for calculating $\mathsf{W}_0[\varphi;1]$ from its large s-behaviour. In this approach, we exploit the analytic structure of $\mathsf{W}_0[\varphi\,;s]$ together with Cauchy's theorem to express $\mathsf{W}_0[\varphi;s]\big|_{s=1} = \mathsf{W}_0[\varphi]$ in terms of its behaviour for large s, using the same contour integral representation introduced in (2.1):

$$\mathsf{W}_0[\varphi] = \lim_{\lambda\to\infty} F[\varphi;\lambda]\,, \qquad F[\varphi;\lambda] = \frac{1}{2\pi i}\int_C \frac{e^{\lambda(s-1)}}{(s-1)}\,\mathsf{W}_0[\varphi\,;s]\,ds\,, \tag{5.186}$$

where C is a very large incomplete circle, centred on the origin in the complex s-plane, beginning just below the negative real axis and ending just above as depicted in Fig.(2.1). The integral in (5.186) is evaluated by deforming the contour C to a small circle around $s=1$, giving $\mathsf{W}_0[\varphi\,;1] = \mathsf{W}_0[\varphi]$, and a keyhole shaped contour C_k, see Fig.(2.2), surrounding the cut on the negative real axis. In the limit as $\lambda\to\infty$, the contribution from

integrating over C_k is exponentially suppressed, in which case we obtain (5.186). In practice, the exact form of $\mathsf{W}_0[\varphi]$ is not known to us. However, we can still employ (5.186) to approximate $\mathsf{W}_0[\varphi]$ by $F[\varphi\,;\lambda]$ for a properly chosen value of λ (say $\lambda = \lambda_e$), using the large s-functional expansion of $\mathsf{W}_0[\varphi\,;s]$ whose analytic structure in the complex s-plane remains unaltered, due to the local[2] nature of this expansion. The proof of the existence of such a local expansion is part of our objectives for the current section.

To see the role of this type of expansion, valid only for fields whose Fourier transforms $\widetilde{\varphi}(k)$ have small compact supports, in constructing $\mathsf{W}_0[\varphi]$ for arbitrary source fields, we begin by considering the Taylor functional expansion of $\mathsf{W}_0[\varphi]$ around $\varphi(x) = 0$:

$$\mathsf{W}_0[\varphi] = \sum_{n=1}^{\infty} \int_{\mathbb{R}} dx_1 \dots dx_n \; G_c^{(n)}(x_1, x_2, \dots, x_n)\; \varphi(x_1)\varphi(x_2)\dots\varphi(x_n)\,, \tag{5.187}$$

where $G_c^{(n)}(x_1, x_2, \dots, x_n)$ is the connected n-point Green's function given by:

$$G_c^{(n)}(x_1, x_2, \dots, x_n) = \frac{1}{n!}\; \frac{\delta^n\, \mathsf{W}_0[\varphi]}{\delta\varphi(x_1)\dots\delta\varphi(x_n)}\bigg|_{\varphi=0}\,. \tag{5.188}$$

Here, $\mathsf{W}_0[\varphi]$ is normalized such that $\mathsf{W}_0[0] = 0$. It follows from (5.188) that $G_c^{(n)}(x_1, \dots, x_n)$ is symmetric in its arguments $x_1, \dots, x_n$. In momentum space, $\mathsf{W}_0[\varphi]$ reads as:

$$\overline{\mathsf{W}}_0[\widetilde{\varphi}] = 2\pi \sum_{n=1}^{\infty} \int_{\mathbb{R}} \Big[\prod_{i=1}^{n} \frac{dk_i}{2\pi}\; \widetilde{\varphi}(k_i)\Big]\; \widetilde{G}_c^{(n)}(k_1, k_2, \dots, k_n)\, \delta(k_1 + \dots + k_n)\,, \tag{5.189}$$

where $\widetilde{G}_c^{(n)}(k_1, k_2, \dots, k_n)$ is the connected n-point Green's function in momentum space, defined by:

$$2\pi\, \widetilde{G}_c^{(n)}(k_1, \dots, k_n)\, \delta(k_1 + \dots + k_n) = \int_{\mathbb{R}} dx_1 \dots dx_n \; G_c^{(n)}(x_1, \dots, x_n)\, \mathrm{e}^{i(k_1x_1 + \dots + k_nx_n)}. \tag{5.190}$$

Note that due to the spatial translation invariance $G_c^{(n)}(x_1, \dots, x_n) = G_c^{(n)}(x_1 + \bar{x}, \dots, x_n + \bar{x})$, the total momentum $\sum k_i$ is conserved, and thus the momentum-conserving delta function in (5.189) is imposed as a constraint on the n momentum variables. The existence of a Taylor expansion of $\widetilde{G}_c^{(n)}(k_1, \dots, k_n)$ in the neighbourhood of the origin $(k_1, \dots, k_n) =$

[2] By "local expansion" we mean that the expansion involves the field φ and a finite number of its derivatives at the same spatial point.

$(0,\ldots,0)$ allows us to rewrite (5.187), for any field $\varphi(x)$ whose Fourier transform $\widetilde{\varphi}(k)$ has a compact support of a sufficiently small size interval, as a single spatial integral of a sum of terms each composed of $\varphi(x)$ and/or a finite number of its derivatives at the same spatial point:

$$\mathsf{W}_0[\varphi] = \sum_{n=1}^{\infty} \sum_{j_1,\ldots,j_n=0}^{\infty} C_{j_1,\ldots,j_n} \int_{\mathbb{R}} dx \; \partial_x^{j_1}\varphi(x)\ldots\partial_x^{j_n}\varphi(x)\,, \tag{5.191}$$

where $C_{j_1,\ldots,j_n}$ denotes constant coefficients. We shall prove this later for any scalar field theory with a non-zero mass gab. Now, under the scale transformation of the source field $\varphi \to \varphi_s = \varphi(x/\sqrt{s})$, with s being real and positive, and a follow-up change of variables $x \to x/\sqrt{s}$, the local functional expansion of $\mathsf{W}_0[\varphi]$ transforms to:

$$\mathsf{W}_0[\varphi_s] = \mathsf{W}_0[\varphi;s] = \sqrt{s} \sum_{n=1}^{\infty} \sum_{j_1,\ldots,j_n=0}^{\infty} \frac{C_{j_1,\ldots,j_n}}{s^{(j_1+\ldots+j_n)/2}} \int_{\mathbb{R}} dx \; \partial_x^{j_1}\varphi(x)\ldots\partial_x^{j_n}\varphi(x)\,, \tag{5.192}$$

Note that for sufficiently large s, i.e. $s \gg 1$, we may truncate this expansion to a good approximation by retaining only the dominant leading terms. From (5.192), we can see clearly that $\mathsf{W}_0[\varphi;s]$ extends to an analytic function of s on the whole of the complex s-plane with a branch cut restricted to the negative real axis. This is a general property of any local functional expansion scaled as in (5.192). Although the local expansion of $\mathsf{W}_0[\varphi]$ is valid only for fields whose Fourier transforms are characterised by sufficiently small supports, it can be used successfully in (5.186) to approximate $\mathsf{W}_0[\varphi]$ for any arbitrary field φ. Let us illustrate this with a specific example. Consider a free massive scalar field theory in 1+1 dimensions in which the logarithm of the vacuum functional assumes the simple form:

$$\mathsf{W}_0[\varphi] = -\frac{1}{2}\int_{\mathbb{R}} dx \; \varphi(x)\,(-\partial_x^2 + m^2)^{1/2}\,\varphi(x)\,. \tag{5.193}$$

For any field $\varphi(x)$ subject to the constraint $|\partial_x\,\varphi(x)| < m|\varphi(x)|$, the following expansion:

$$(-\partial_x^2 + m^2)^{1/2}\,\varphi(x) = \frac{\sqrt{\pi}}{2} \sum_{n=0}^{\infty} \frac{(-1)^n\, m^{-2n+1}}{\Gamma(n+1)\Gamma(3/2-n)}\,\partial_x^{2n}\,\varphi(x)\,, \tag{5.194}$$

is convergent, and when used in (5.193) gives:

$$\mathsf{W}_0[\varphi] = \sum_{n=0}^{\infty} a_n \int_{\mathbb{R}} dx\ \varphi(x)\, \partial_x^{2n} \varphi(x)\,, \qquad a_n = -\frac{\sqrt{\pi}\,(-1)^n\, m^{-2n+1}}{4\,\Gamma(n+1)\Gamma(3/2-n)}\,. \tag{5.195}$$

This reflects the local character of $\mathsf{W}_0[\varphi]$ in the free scalar field theory, which holds only for fields whose Fourier transforms $\widetilde{\varphi}(k)$ vanish for momenta with magnitude greater than the mass m. By substituting the scaled field $\varphi_s = \varphi(x/\sqrt{s})$ for $\varphi(x)$ in (5.195), and then making the dependence on s more explicit by letting $x \to x/\sqrt{s}$ we obtain:

$$\mathsf{W}_0[\varphi_s] = \mathsf{W}_0[\varphi; s] = \sum_{n=0}^{\infty} \frac{a_n\, I_n[\varphi]}{s^{n-1/2}}\,, \qquad I_n[\varphi] = \int_{\mathbb{R}} dx\ \varphi(x)\, \partial_x^{2n} \varphi(x)\,, \tag{5.196}$$

which is now subject to the constraint $|\partial_x\, \varphi(x)| < \sqrt{s}\, m\, |\varphi(x)|$. This expression allows the analytic continuation to complex values of s, yielding a function of s that is analytic on the complex s-plane with the negative real axis removed. To express $\mathsf{W}_0[\varphi] = \mathsf{W}_0[\varphi; 1]$ in terms of its value for large s we substitute (5.196) into the contour integral (5.186), giving:

$$F[\varphi; \lambda] = \sum_{n=0}^{\infty} a_n\, I_n[\varphi]\, f_n(\lambda)\,, \tag{5.197}$$

where

$$f_n(\lambda) = \frac{1}{2\pi i} \int_C \frac{ds}{s^{n-1/2}}\, \frac{\mathrm{e}^{\lambda(s-1)}}{(s-1)}\,, \qquad \lambda > 0\,. \tag{5.198}$$

With the help of Cauchy's theorem, we can deform the large incomplete circle C in (5.198) to a small circle around $s = 1$ and a keyhole shaped contour C_k, see Fig.(2.2), surrounding the cut on the negative real axis. This allows us to write:

$$f_n(\lambda) = 1 + \frac{1}{2\pi i} \int_{C_k} \frac{ds}{s^{n-1/2}}\, \frac{\mathrm{e}^{\lambda(s-1)}}{(s-1)}\,. \tag{5.199}$$

Making use of the fact that:

$$\frac{1}{s-1} = -\int_0^{\infty} dt\ \mathrm{e}^{t(s-1)}\,, \qquad \text{for all } s \text{ on } C_k\,, \tag{5.200}$$

gives:

$$f_n(\lambda) = 1 - \frac{\mathrm{e}^{-\lambda}}{2\pi i} \int_{C_k} ds \int_0^{\infty} dt\ \frac{\mathrm{e}^{s(\lambda+t)-t}}{s^{n-1/2}}\,. \tag{5.201}$$

Since the t-integral in this expression converges uniformly for all values of s on C_k, the order of integration can be interchanged, allowing us to integrate over C_k first which is known to be:

$$\int_{C_k} ds \; \frac{e^{s(\lambda+t)}}{s^{n-1/2}} = 2\pi i \, \frac{(t+\lambda)^{n-3/2}}{\Gamma(n-1/2)} \,. \tag{5.202}$$

From this, it follows that:

$$f_n(\lambda) = 1 - \frac{e^{-\lambda}}{\Gamma(n-1/2)} \int_0^\infty dt \; \frac{e^{-t}}{(t+\lambda)^{3/2-n}} \,. \tag{5.203}$$

Making the change of variables $t \to t + \lambda$ reduces (5.203) to:

$$f_n(\lambda) = 1 - \frac{\Gamma(n-1/2, \lambda)}{\Gamma(n-1/2)} \,, \tag{5.204}$$

where $\Gamma(\alpha, \lambda)$ is the incomplete Gamma function, defined by [28]:

$$\Gamma(\alpha, \lambda) = \int_\lambda^\infty e^{-t} \; t^{\alpha-1} \, dt \,. \tag{5.205}$$

Now, if we substitute (5.204) into (5.197) we obtain:

$$F[\varphi; \lambda] = W_0[\varphi] - \sum_{n=0}^{\infty} a_n \, I_n[\varphi] \, \frac{\Gamma(n-1/2, \lambda)}{\Gamma(n-1/2)} \,, \tag{5.206}$$

which tends to $W_0[\varphi]$ as $\lambda \to \infty$. So far, we have considered the case in which we know the exact expansion of $W_0[\varphi]$ for a field φ whose Fourier transform $\widetilde{\varphi}(k)$ is non-zero only for small momenta. In practice, however, we do only know this within the limits of perturbation theory. Thus, letting $\lambda \to \infty$ in this case would simply reproduce the original perturbative expansion of $W_0[\varphi]$, leading to nothing new. So, if instead of using the limiting value of $F[\varphi; \lambda]$ we were to use a finite value of λ, say λ_e, then we would have an expression that includes the perturbative part of the expansion and a correction term depending on λ_e. In this way, we obtain an approximation method for expanding the region of applicability of the truncated local expansion.

In conclusion, although local expansions of functionals of the type (5.191) are valid only for source fields with Fourier transforms $\widetilde{\varphi}(k)$ restricted to sufficiently small supports, we can still exploit their analytic structure under a scale transformation of the source fields,

$\varphi \to \varphi_s = \varphi(x/\sqrt{s})$, to reconstruct their behaviour for arbitrary fields. Thus, a knowledge of these local expansions in field theories are sufficient in our approach to estimate the vacuum functional of an arbitrary source field.

Having discussed the major role played in obtaining $W_0[\varphi]$ for arbitrary fields by the local expansion of $W_0[\varphi]$ and its analytic properties under complex scaling, we shall now investigate the existence of this expansion in a 2-dimensional interacting scalar field theory with a non-zero mass gap. Also, we shall study the analyticity of W_0 for a scaled field $\varphi_s = \varphi(x/\sqrt{s})$, showing that it extends to an analytic function of s in the complex s-plane with the negative real axis removed.

Consider the Euclidean path integral representation (5.128) for the Schrödinger vacuum functional, written in 1+1 dimension as:

$$\Psi_0[\varphi] = N \int_{\phi=0}^{\phi=0} \mathcal{D}\phi \, \exp\Big(- S_E[\phi] - \int_{-\infty}^{\infty} dx \, \varphi(x) \, \dot{\phi}(x,0) \Big). \tag{5.207}$$

Here, we have ignored the singular term $\delta(0) \int_{-\infty}^{\infty} dx \, \varphi^2(x)$ in the exponent of (5.128) since it amounts to a source counter term which can be added when renormalizing. Now, by rotating the Euclidean space-time coordinates according to:

$$\begin{pmatrix} x \\ t \end{pmatrix} \to \begin{pmatrix} x_r \\ t_r \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ t \end{pmatrix}, \tag{5.208}$$

such that $x_r = -t \geq 0$ and $t_r = x \in \mathbb{R}$, we obtain:

$$\Psi_0[\varphi] = N_r \int_{\phi_r=0}^{\phi_r=0} \mathcal{D}\phi_r \, \exp\Big(- S_E^r[\phi_r] + \int_{-\infty}^{\infty} dt_r \, \varphi(t_r) \, \phi_r'(0,t_r) \Big), \tag{5.209}$$

where $\phi_r(x_r,t_r) = \phi(x,t)$, satisfying the boundary conditions $\phi_r(0,t_r) = \phi_r(\infty,t_r) = 0$, and the prime in ϕ_r' denotes differentiation with respect to the spatial coordinate x_r. Here, N_r normalizes Ψ_0 to unity, i.e. $\Psi_0[0] = 1$, and $S_E^r[\phi_r]$ signifies the Euclidean action in the new rotated system of coordinates:

$$S_E^r[\phi_r] = \int_{-\infty}^{\infty} dt_r \int_0^{\infty} dx_r \; \mathcal{L}^r(\phi_r, \dot{\phi}_r), \tag{5.210}$$

with the interacting Lagrangian density:

$$\mathcal{L}^r = \frac{1}{2}\left(\dot{\phi}_r^2 + \phi'^2_r + m^2\,\phi_r^2\right) + g\,\mathcal{H}_1(\phi_r)\,. \tag{5.211}$$

In the canonical formalism, the functional integral in (5.209) is interpreted as the vacuum expectation value of the time-ordered exponential $\exp\left(\int_{-\infty}^{\infty} dt_r\ \varphi(t_r)\,\hat{\phi}'_r(0,t_r)\right)$, namely:

$$\Psi_0[\varphi] = \langle 0_r|\,\mathbf{T}\exp\left(\int_{-\infty}^{\infty} dt_r\ \varphi(t_r)\,\hat{\phi}'_r(0,t_r)\right)|0_r\rangle\,, \tag{5.212}$$

where the time-dependent field operator $\hat{\phi}'_r(0,t_r)$ is defined in the Euclidean interaction picture as:

$$\hat{\phi}'_r(0,t_r) = \mathrm{e}^{t_r\widehat{H}_r}\ \hat{\phi}'_r(0,0)\ \mathrm{e}^{-t_r\widehat{H}_r}\,, \tag{5.213}$$

with $\widehat{H}_r$ being the time-independent Hamiltonian of the Euclidean rotated theory characterised by the action S_E^r in (5.210). Here, $|0_r\rangle$ is the ground state of $\widehat{H}_r$ with zero energy eigenvalue, i.e. $\widehat{H}_r|0_r\rangle = 0$. The time-dependent source $\varphi(t_r)$ is assumed to be adiabatically switched off in the remote past and the distant future, i.e. near $t_r = \pm\infty$. By expanding the exponential in (5.212) and then Fourier transforming the source fields and using (5.213) in this expansion, we arrive at:

$$\begin{aligned}\Psi_0[\varphi] = \overline{\Psi}_0[\widetilde{\varphi}] = \sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\cdots\frac{dk_n}{2\pi}\ \widetilde{\varphi}(k_1)\,\widetilde{\varphi}(k_1)\ldots\widetilde{\varphi}(k_n)\\ \times\int_{-\infty}^{\infty}dt_n\int_{-\infty}^{t_n}dt_{n-1}\cdots\int_{-\infty}^{t_2}dt_1\ \mathrm{e}^{i(k_1t_1+k_2t_2+\cdots+k_nt_n)}\\ \times\langle 0_r|\hat{\phi}'_r(0,0)\,\mathrm{e}^{-(t_n-t_{n-1})\widehat{H}_r}\hat{\phi}'_r(0,0)\ldots\ldots\hat{\phi}'_r(0,0)\,\mathrm{e}^{-(t_2-t_1)\widehat{H}_r}\hat{\phi}'_r(0,0)|0_r\rangle\,.\end{aligned} \tag{5.214}$$

By inserting a complete set of eigenstates of $\widehat{H}_r$, namely $\sum_{\ell\in\mathbb{N}}|E_\ell\rangle\langle E_\ell| = 1$ with $|E_0\rangle = |0_r\rangle$, in front of each exponential operator in (5.214), and then performing all the t_i-integrations, we obtain:

$$\overline{\Psi}_0[\widetilde{\varphi}] = 1 + \sum_{n=1}^{\infty}\overline{\Psi}_0^{(n)}[\widetilde{\varphi}]\,, \tag{5.215}$$

where

$$\overline{\Psi}_0^{(n)}[\widetilde{\varphi}] = 2\pi\int_{-\infty}^{\infty}\left[\prod_{i=1}^{n}\frac{dk_i}{2\pi}\ \widetilde{\varphi}(k_i)\right]\widetilde{\mathfrak{J}}_d^{(n)}(k_1,\ldots,k_n)\,\delta(k_1+\cdots+k_n)\,. \tag{5.216}$$

Here, the disconnected n-point Green's function $\widetilde{\mathfrak{J}}_d^{(n)}(k_1,\ldots,k_n)$ in rotated space is given by:

$$\widetilde{\mathfrak{J}}_d^{(n)}(k_1,\ldots,k_n) = \sum_{\ell_1=0}^{\infty}\sum_{\ell_2=0}^{\infty}\cdots\sum_{\ell_{n-1}=0}^{\infty} \frac{\Big[\prod_{j=0}^{n-1}\Omega(\ell_j,\ell_{j+1})\Big]\Big|_{\ell_0=0}^{\ell_n=0}}{\prod_{j=1}^{n-1}\big(E_{\ell_j}+i\,\overline{k}_{n-j}\big)}\,, \tag{5.217}$$

where $\overline{k}_\ell = k_1+k_2+\cdots+k_\ell$ with $\overline{k}_n = 0$ representing the δ-function constraint in (5.216), and:

$$\Omega(\ell_j,\ell_{j+1}) = \langle E_{\ell_j}|\hat{\phi}_r'(0,0)|E_{\ell_{j+1}}\rangle\,. \tag{5.218}$$

Without any loss of generality in our argument, we assume that:

$$\Omega(0,0) = \langle E_0|\hat{\phi}_r'(0,0)|E_0\rangle = 0 \implies \widetilde{\mathfrak{J}}_d^{(1)}(k_1) = 0\,. \tag{5.219}$$

This is always true for any field theory that is invariant under the symmetry transformation $\varphi(x)\to-\varphi(x)$, such as the φ^{2n}–theories with $n\in\mathbb{N}$. To justify the use of (5.219) for other field theories, say those of the type φ^{2n+1}, we apply the change of variables:

$$\phi_r(x,t)\to\eta(x,t) = \phi_r(x,t) - \langle E_0|\hat{\phi}_r(x,0)|E_0\rangle\,, \tag{5.220}$$

to the functional integral (5.209) in which case we obtain in the canonical formalism:

$$\Psi_0[\varphi] = \mathrm{e}^{\Omega(0,0)\bar{\varphi}(0)}\ \langle 0_r|\,\mathbf{T}\exp\Big(\int_{-\infty}^{\infty}dt_r\ \varphi(t_r)\,\hat{\eta}'(0,t_r)\Big)\,|0_r\rangle\,. \tag{5.221}$$

Starting with this expression, we can show that $\langle 0_r|\mathbf{T}\exp\big(\int dt_r\varphi(t_r)\,\hat{\eta}'(0,t_r)\big)|0_r\rangle$ has the same n-point Green's function as $\widetilde{\mathfrak{J}}_d^{(n)}(k_1,\ldots,k_n)$ with the constant coefficients $\Omega(\ell,\ell')$ in (5.218) replaced by:

$$\widetilde{\Omega}(\ell,\ell') = \langle E_\ell|\hat{\eta}'(0,0)|E_{\ell'}\rangle = \langle E_\ell|\hat{\phi}_r'(0,0)|E_{\ell'}\rangle - \langle E_0|\hat{\phi}_r'(0,0)|E_0\rangle\,\delta_{\ell\ell'}\,, \tag{5.222}$$

which illustrates that $\widetilde{\Omega}(0,0) = 0$. Therefore, our forthcoming argument will not be affected by adopting (5.219).

To simplify the presentation of our calculations, we shall from now on employ the

following notations:

$$\triangle^{(n_j)}(\widetilde{\mathfrak{m}}_j) = \prod_{\ell=0}^{n_j-1} \Omega(\mathfrak{m}_{\overline{n}_{j-1}+\ell}, \mathfrak{m}_{\overline{n}_{j-1}+\ell+1})\Big|_{\mathfrak{m}_{\overline{n}_{j-1}}=0}^{\mathfrak{m}_{\overline{n}_j}=0}, \qquad \text{for } j = 1, 2\ldots, \tag{5.223}$$

where n_j is a positive integer greater than 1, $\overline{n}_j = n_1 + n_2 + \cdots + n_j$ with $\overline{n}_0 = 0$ and $\widetilde{\mathfrak{m}}_j$ denotes the sequence:

$$\widetilde{\mathfrak{m}}_j = \{\mathfrak{m}_{\overline{n}_{j-1}+\ell}\}_{\ell=1}^{\ell=n_j-1} = \mathfrak{m}_{\overline{n}_{j-1}+1}, \mathfrak{m}_{\overline{n}_{j-1}+2}, \ldots, \mathfrak{m}_{\overline{n}_j-1}, \qquad \mathfrak{m}_\ell \in \mathbb{N}. \tag{5.224}$$

As an example, for $j = 1$ and 2 we have:

$$\triangle^{(n_1)}(\widetilde{\mathfrak{m}}_1) = \triangle^{(n_1)}(\mathfrak{m}_1, \mathfrak{m}_2, \ldots, \mathfrak{m}_{n_1-1}) = \prod_{\ell=0}^{n_1-1} \Omega(\mathfrak{m}_\ell, \mathfrak{m}_{\ell+1})\Big|_{\mathfrak{m}_0=0}^{\mathfrak{m}_{n_1}=0}, \tag{5.225}$$

$$\triangle^{(n_2)}(\widetilde{\mathfrak{m}}_2) = \triangle^{(n_2)}(\mathfrak{m}_{n_1+1}, \ldots, \mathfrak{m}_{n_1+n_2-1}) = \prod_{\ell=0}^{n_2-1} \Omega(\mathfrak{m}_{n_1+\ell}, \mathfrak{m}_{n_1+\ell+1})\Big|_{\mathfrak{m}_{n_1}=0}^{\mathfrak{m}_{n_1+n_2}=0}. \tag{5.226}$$

By definition, we shall take:

$$\triangle^{(n_j)}(\widetilde{\mathfrak{m}}_j) = 0 \qquad \text{for any} \quad n_j < 2\,. \tag{5.227}$$

For brevity the bar on any indexed variable, say $\overline{q}_\ell$, will always mean a summation over the variable index running from 1 to ℓ, i.e. $\overline{q}_\ell = q_1 + \cdots + q_\ell$ with $\overline{q}_0 = 0$. Using these notations, let us now rearrange the expansion of $\widetilde{\mathfrak{J}}_d^{(n)}(k_1, \ldots, k_n)$ in (5.217) according to the vacuum energy contributions, rewriting (5.217) as:

$$\widetilde{\mathfrak{J}}_d^{(n)}(k_1, \ldots, k_n) = \sum_{r=1}^{[n]} \widetilde{\mathfrak{J}}_d^{(n,r)}(k_1, \ldots, k_n)\,, \qquad [n] = \begin{cases} \frac{n}{2} & \text{if } n \text{ is even} \\ \frac{n-1}{2} & \text{if } n \text{ is odd}\,, \end{cases} \tag{5.228}$$

where $\widetilde{\mathfrak{J}}_d^{(n,r)}(k_1, \ldots, k_n)$ denotes all the terms in the expansion of (5.217) with $r-1$ vacuum

energy contributions:

$$\widetilde{\mathfrak{J}}_d^{(n,1)}(k_1,\ldots,k_n) = \sum_{\mathfrak{m}_1=1}^{\infty}\sum_{\mathfrak{m}_2=1}^{\infty}\cdots\sum_{\mathfrak{m}_{n-1}=1}^{\infty} \frac{\triangle^{(n)}(\mathfrak{m}_1,\mathfrak{m}_2,\ldots,\mathfrak{m}_{n-1})}{\prod_{\ell=1}^{n-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)}\,, \tag{5.229}$$

$$\widetilde{\mathfrak{J}}_d^{(n,2)}(k_1,\ldots,k_n) = \sum_{n_1=2}^{n-2}\Big[\prod_{\substack{\ell=1\\ \ell\neq n_1}}^{n-1}\sum_{\mathfrak{m}_\ell=1}^{\infty}\Big]\triangle^{(n_1)}(\mathfrak{m}_1,\ldots,\mathfrak{m}_{n_1-1})\,\triangle^{(n-n_1)}(\mathfrak{m}_{n_1+1},\ldots,\mathfrak{m}_{n-1})$$
$$\times\ \frac{1}{(\epsilon+i\,\overline{k}_{n-n_1})\prod_{\substack{\ell=1\\ \ell\neq n_1}}^{n-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)}\,, \tag{5.230}$$

$$\vdots$$

$$\widetilde{\mathfrak{J}}_d^{(n,r)}(k_1,\ldots,k_n) = \sum_{\substack{n_1,\ldots,n_r=2\\ n_1+\cdots+n_r=n}}^{n-2(r-1)}\sum_{\{\widetilde{\mathfrak{m}}_1\}}\sum_{\{\widetilde{\mathfrak{m}}_2\}}\cdots\sum_{\{\widetilde{\mathfrak{m}}_r\}}\triangle^{(n_1)}(\widetilde{\mathfrak{m}}_1)\,\triangle^{(n_2)}(\widetilde{\mathfrak{m}}_2)\ldots\triangle^{(n_r)}(\widetilde{\mathfrak{m}}_r)$$
$$\times\ \frac{1}{\Big[\prod_{j=1}^{r-1}\left(\epsilon_j+i\,\overline{k}_{n-\overline{n}_j}\right)\Big]\Big[\prod_{\ell\notin\{\overline{n}_1,\ldots,\overline{n}_{r-1}\}}^{n-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)\Big]}\,, \tag{5.231}$$

where the infinitesimally small positive constants ϵ_j are used in place of the zero vacuum energy E_0 in order to regularise $\widetilde{\mathfrak{J}}_d^{(n,r)}(k_1,\ldots,k_n)$ at the origin $(k_1,\ldots,k_n)=(0,\ldots,0)$. Here, the sum $\sum_{\{\widetilde{\mathfrak{m}}_j\}}$ and the restricted product of $X_\ell=(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell})$ are defined as:

$$\sum_{\{\widetilde{\mathfrak{m}}_j\}} = \prod_{\ell=\overline{n}_{j-1}+1}^{\overline{n}_j-1}\sum_{\mathfrak{m}_\ell=1}^{\infty}\,,\qquad \prod_{\ell\notin\{\overline{n}_1,\ldots,\overline{n}_{r-1}\}}^{n-1}X_\ell = \prod_{j=1}^{r}\Big[\prod_{\ell_j=\overline{n}_{j-1}+1}^{\overline{n}_j-1}X_{\ell_j}\Big]\,. \tag{5.232}$$

Note that $\widetilde{\mathfrak{J}}_d^{(n,r)}(k_1,\ldots,k_n)=0$ for $n=1$. Now we shall use (5.231) to redefine $\overline{\Psi}_0^{(n)}[\widetilde{\varphi}]$ in (5.216), giving:

$$\overline{\Psi}_0^{(n)}[\widetilde{\varphi}] = \sum_{r=1}^{[n]}\overline{\Psi}_0^{(n,r)}[\widetilde{\varphi}]\,, \tag{5.233}$$

where

$$\overline{\Psi}_0^{(n,r)}[\widetilde{\varphi}] = 2\pi\int_{-\infty}^{\infty}\Big[\prod_{i=1}^{n}\frac{dk_i}{2\pi}\ \widetilde{\varphi}(k_i)\Big]\,\widetilde{\mathfrak{J}}_d^{(n,r)}(k_1,\ldots,k_n)\,\delta(k_1+\cdots+k_n)\,. \tag{5.234}$$

The logarithm of (5.215) reads as:

$$\overline{\mathsf{W}}_0[\widetilde{\varphi}] = \sum_{n=1}^{\infty} \overline{\mathsf{W}}_0^{(n)}[\widetilde{\varphi}]\,, \tag{5.235}$$

where

$$\overline{\mathsf{W}}_0^{(n)}[\widetilde{\varphi}] = \sum_{\jmath=1}^{[n]} \sum_{\substack{n_1,\dots,n_\jmath=2 \\ n_1+\cdots+n_\jmath=n}}^{n-2(\jmath-1)} \frac{(-1)^{\jmath-1}}{\jmath} \prod_{\imath=1}^{\jmath} \overline{\Psi}_0^{(n_\imath)}[\widetilde{\varphi}] = \overline{\Psi}_0^{(n)}[\widetilde{\varphi}] - \frac{1}{2}\sum_{n_1=2}^{n-2} \overline{\Psi}_0^{(n_1)}[\widetilde{\varphi}]\,\overline{\Psi}_0^{(n-n_1)}[\widetilde{\varphi}]$$
$$+ \frac{1}{3}\sum_{n_1=2}^{n-4}\sum_{n_2=2}^{n-4} \overline{\Psi}_0^{(n_1)}[\widetilde{\varphi}]\,\overline{\Psi}_0^{(n_2)}[\widetilde{\varphi}]\,\overline{\Psi}_0^{(n-(n_1+n_2))}[\widetilde{\varphi}] + \dots\,. \tag{5.236}$$

This expansion can be rearranged according to the vacuum energy contributions, giving:

$$\overline{\mathsf{W}}_0^{(n)}[\widetilde{\varphi}] = \sum_{r=1}^{[n]} \overline{\mathsf{W}}_0^{(n,r)}[\widetilde{\varphi}]\,, \tag{5.237}$$

where

$$\overline{\mathsf{W}}_0^{(n,1)}[\widetilde{\varphi}] = \overline{\Psi}_0^{(n,1)}[\widetilde{\varphi}]\,, \tag{5.238}$$

$$\overline{\mathsf{W}}_0^{(n,2)}[\widetilde{\varphi}] = \overline{\Psi}_0^{(n,2)}[\widetilde{\varphi}] - \frac{1}{2}\sum_{n_1=2}^{n-2} \overline{\Psi}_0^{(n_1,1)}[\widetilde{\varphi}]\,\overline{\Psi}_0^{(n-n_1,1)}[\widetilde{\varphi}]\,, \tag{5.239}$$

$$\overline{\mathsf{W}}_0^{(n,3)}[\widetilde{\varphi}] = \overline{\Psi}_0^{(n,3)}[\widetilde{\varphi}] - \sum_{n_1=2}^{n-4} \overline{\Psi}_0^{(n_1,1)}[\widetilde{\varphi}]\,\overline{\Psi}_0^{(n-n_1,2)}[\widetilde{\varphi}]$$
$$+ \frac{1}{3}\sum_{n_1=2}^{n-4}\sum_{n_2=2}^{n-4} \overline{\Psi}_0^{(n_1,1)}[\widetilde{\varphi}]\,\overline{\Psi}_0^{(n_2,1)}[\widetilde{\varphi}]\,\overline{\Psi}_0^{(n-(n_1+n_2),1)}[\widetilde{\varphi}]\,, \tag{5.240}$$

$$\vdots$$

$$\overline{\mathsf{W}}_0^{(n,r)}[\widetilde{\varphi}] = \sum_{\jmath=1}^{r} \frac{(-1)^{\jmath-1}}{\jmath} \sum_{\substack{n_1,\dots,n_\jmath=2 \\ n_1+\cdots+n_\jmath=n}}^{n-2(\jmath-1)} \left[\prod_{\imath=1}^{\jmath}\sum_{r_\imath=1}^{[n_\imath]} \overline{\Psi}_0^{(n_\imath,r_\imath)}[\widetilde{\varphi}]\right] \delta_{r_1+\cdots+r_\jmath,r}\,. \tag{5.241}$$

In what follows, we shall show that the connected n-point Green's functions in momentum space $\widetilde{G}_c^{(n)}(k_1,\dots,k_n)$ are analytic around the origin $(k_1,\dots,k_n) = (0,\dots,0)$ and can be Taylor expanded over a small domain provided that the theory has a non-zero mass gap. This proof requires the cancellation of all the denominators associated with the zero-point energy in $\widetilde{\mathfrak{J}}_d^{(n,r)}(k_1,\dots,k_n)$, which is a highly non-trivial task but it can be verified

explicitly order by order in r through some laborious calculations. Our proof will cover only the n-point functions associated with $\overline{\mathsf{W}}_0^{(n,r)}[\widetilde{\varphi}]$ for $r \leq 3$. This will include the entire vacuum energy expansion of each function $\widetilde{G}_c^{(n)}(k_1, \ldots, k_n)$ with $n \leq 7$.

From (5.189) and (5.237), it follows that:

$$\widetilde{G}_c^{(n)}(k_1, \ldots, k_n) = \sum_{r=1}^{[n]} \widetilde{G}_c^{(n,r)}(k_1, \ldots, k_n)\,, \tag{5.242}$$

with $\widetilde{G}_c^{(n,r)}(k_1, \ldots, k_n)$ being associated with $\overline{\mathsf{W}}_0^{(n,r)}[\widetilde{\varphi}]$ as:

$$\overline{\mathsf{W}}_0^{(n,r)}[\widetilde{\varphi}] = 2\pi \int_{\mathbb{R}} \Big[\prod_{i=1}^{n} \frac{dk_i}{2\pi}\, \widetilde{\varphi}(k_i)\Big]\, \widetilde{G}_c^{(n,r)}(k_1, \ldots, k_n)\, \delta(k_1 + \cdots + k_n)\,. \tag{5.243}$$

Since $\overline{\mathsf{W}}_0^{(n,1)}[\widetilde{\varphi}] = \overline{\Psi}_0^{(n,1)}[\widetilde{\varphi}]$, we deduce from (5.231) and (5.234) that

$$\widetilde{G}_c^{(n,1)}(k_1, \ldots, k_n) = \sum_{\mathsf{m}_1=1}^{\infty} \sum_{\mathsf{m}_2=1}^{\infty} \cdots \sum_{\mathsf{m}_{n-1}=1}^{\infty} \frac{\triangle^{(n)}(\mathsf{m}_1, \mathsf{m}_2, \ldots, \mathsf{m}_{n-1})}{\prod_{\ell=1}^{n-1} \big(E_{\mathsf{m}_\ell} + i\,\overline{k}_{n-\ell}\big)}\,, \tag{5.244}$$

which is Taylor expandable in the neighbourhood of the origin in the n-dimensional k-space. This is because the denominator in (5.244) does not include any zero energy value that would otherwise have made $\widetilde{G}_c^{(n,1)}$ singular at the origin. Let us now prove that this is also the case for $\widetilde{G}_c^{(n,2)}(k_1, \ldots, k_n)$.

Using (5.234) for $r = 2$ in expression (5.239) gives:

$$\begin{aligned}
\overline{\mathsf{W}}_0^{(n,2)}[\widetilde{\varphi}] = {} & 2\pi \int_{\mathbb{R}} \Big[\prod_{i=1}^{n} \frac{dk_i}{2\pi}\, \widetilde{\varphi}(k_i)\Big]\, \widetilde{\mathfrak{J}}_d^{(n,2)}(k_1, \ldots, k_n)\, \delta(k_1 + \cdots + k_n) \\
& - 2\pi^2 \sum_{n_1=2}^{n-2} \int_{\mathbb{R}} \Big[\prod_{i=1}^{n_1} \frac{dk_i}{2\pi}\, \widetilde{\varphi}(k_i)\Big]\Big[\prod_{i=1}^{n-n_1} \frac{dk'_i}{2\pi}\, \widetilde{\varphi}(k'_i)\Big]\, \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1, \ldots, k_{n_1}) \\
& \times\, \widetilde{\mathfrak{J}}_d^{(n-n_1,1)}(k'_1, \ldots, k'_{n-n_1})\, \delta(k_1 + \cdots + k_{n_1})\, \delta(k'_1 + \cdots + k'_{n-n_1})\,.
\end{aligned} \tag{5.245}$$

By letting $k'_i = k_{n_1+i}$ for $i = 1, 2, \ldots, n - n_1$ and using the fact that:

$$\delta(k_1 + \cdots + k_{n_1})\, \delta(k_{n_1+1} + \cdots + k_n) = \delta(k_1 + \cdots + k_{n_1})\, \delta(k_1 + \cdots + k_n)\,, \tag{5.246}$$

we obtain from (5.245):

$$\widetilde{G}_c^{(n,2)}(k_1,\dots,k_n) = \widetilde{\mathfrak{J}}_d^{(n,2)}(k_1,\dots,k_n) - \pi \sum_{n_1=2}^{n-2} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,\dots,k_{n_1}) \times \widetilde{\mathfrak{J}}_d^{(n-n_1,1)}(k_{n_1+1},\dots,k_n)\,\delta(k_1+\cdots+k_{n_1})\,. \tag{5.247}$$

Let us now try to extract from $\widetilde{\mathfrak{J}}_d^{(n,2)}$ a proper combination of $\widetilde{\mathfrak{J}}_d^{(n_1,1)}$ and $\widetilde{\mathfrak{J}}_d^{(n-n_1,1)}$ that would cancel the $2nd$-term in (5.247), which would otherwise spoil the required local expansion in the lower IR-domain. We begin by making use of the so-called Sokhotski-Plemelj equations [62]:

$$\lim_{\epsilon\to 0} \frac{1}{\epsilon \pm i\,k} = \pi\,\delta(k) \mp i\,\mathrm{P}(1/k), \qquad \mathrm{P}(1/k) = \begin{cases} \dfrac{1}{k} & \text{if } k \neq 0\,, \\ 0 & \text{if } k = 0\,, \end{cases} \tag{5.248}$$

in expression (5.230), rewriting $\widetilde{\mathfrak{J}}_d^{(n,2)}(k_1,\dots,k_n)$ as:

$$\widetilde{\mathfrak{J}}_d^{(n,2)}(k_1,\dots,k_n) = \pi \sum_{n_1=2}^{n-2} \mathfrak{a}_{n_1}\,\mathfrak{b}_{n_1}\,\delta(\overline{k}_{n-n_1}) - i \sum_{n_1=2}^{n-2} \mathfrak{a}_{n_1}\,\mathfrak{b}_{n_1}\,\mathrm{P}\left(\frac{1}{\overline{k}_{n-n_1}}\right), \tag{5.249}$$

where

$$\mathfrak{a}_{n_1} = \sum_{\mathfrak{m}_1=1}^{\infty} \cdots \sum_{\mathfrak{m}_{n_1-1}=1}^{\infty} \frac{\triangle^{(n_1)}(\mathfrak{m}_1,\dots,\mathfrak{m}_{n_1-1})}{\prod_{\ell=1}^{n_1-1} \left(E_{\mathfrak{m}_\ell} + i\,\overline{k}_{n-\ell}\right)}, \tag{5.250}$$

$$\mathfrak{b}_{n_1} = \sum_{\mathfrak{m}_{n_1+1}=1}^{\infty} \cdots \sum_{\mathfrak{m}_{n-1}=1}^{\infty} \frac{\triangle^{(n-n_1)}(\mathfrak{m}_{n_1+1},\dots,\mathfrak{m}_{n-1})}{\prod_{j=n_1+1}^{n-1} \left(E_{\mathfrak{m}_j} + i\,\overline{k}_{n-j}\right)}. \tag{5.251}$$

In (5.250), the set of $n-\ell$ variables in the sum $\overline{k}_{n-\ell} = k_1 + k_2 + \cdots + k_{n-\ell}$ can be divided into two groups $\{k_1, k_2, \dots, k_{n-n_1}\}$ and $\{k_{n-n_1+1}, \dots, k_{n-\ell}\}$, allowing us to write $\overline{k}_{n-\ell} = \overline{k}_{n-n_1} + k_{n-n_1+1} + \cdots + k_{n-\ell}$ which reduces to $\overline{k}_{n-\ell} = k_{n-n_1+1} + \cdots + k_{n-\ell}$ as $\overline{k}_{n-n_1} = 0$ due to the δ-function constraint $\delta(\overline{k}_{n-n_1})$. So, by replacing the sum $\overline{k}_{n-\ell}$ in (5.250) with $\sum_{j=1}^{n_1-\ell} k_{n-n_1+j}$ we deduce from (5.229) that:

$$\mathfrak{a}_{n_1} = \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_{n-n_1+1}, k_{n-n_1+2}, \dots, k_n)\,. \tag{5.252}$$

Also, by substituting $\prod_{j=1}^{n-n_1-1}\left(E_{\mathfrak{m}_{n_1+j}}+i\,\overline{k}_{n-n_1-j}\right)$ for $\prod_{j=n_1+1}^{n-1}\left(E_{\mathfrak{m}_j}+i\,\overline{k}_{n-j}\right)$ in (5.251) we can see from (5.229) that:

$$\mathfrak{b}_{n_1}=\widetilde{\mathfrak{J}}_d^{(n-n_1,1)}(k_1,k_2,\ldots,k_{n-n_1})\,. \tag{5.253}$$

This together with (5.252) and (5.249) allows us to rewrite (5.247) as:

$$\begin{aligned}\widetilde{G}_c^{(n,2)}(k_1,\ldots,k_n)=-i\sum_{n_1=2}^{n-2}\Big[\prod_{\ell=1}^{n_1-1}\sum_{\mathfrak{m}_\ell=1}^{\infty}\Big]\Big[\prod_{\ell'=n_1+1}^{n-1}\sum_{\mathfrak{m}_{\ell'}=1}^{\infty}\Big]\\ \times\frac{\triangle^{(n_1)}(\mathfrak{m}_1,\ldots,\mathfrak{m}_{n_1-1})\,\triangle^{(n-n_1)}(\mathfrak{m}_{n_1+1},\ldots,\mathfrak{m}_{n-1})}{\prod_{\ell=1}^{n_1-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)\prod_{\ell'=n_1+1}^{n-1}\left(E_{\mathfrak{m}_{\ell'}}+i\,\overline{k}_{n-\ell'}\right)}\,\mathrm{P}\left(\frac{1}{\overline{k}_{n-n_1}}\right),\end{aligned} \tag{5.254}$$

At first glance, the Cauchy principal part $\mathrm{P}\big(1/\overline{k}_{n-n_1}\big)$ seems to make the local expansion of $\mathsf{W}_0^{(n,2)}[\varphi]$ unobtainable. This is because it prevents $\widetilde{G}_c^{(n,2)}(k_1,\ldots,k_n)$ from having a Taylor expansion around the origin $(0,0,\ldots,0)$. To overcome this problem, let us make use of the following identity:

$$\begin{aligned}\frac{1}{\prod_{\ell=1}^{n}(a_\ell+i\,x_\ell)}&=\frac{1}{\prod_{\ell=1}^{n}(a_\ell+i\,(x_\ell-b))}\\ &\quad-i\,b\sum_{\nu=1}^{n}\frac{1}{\Big[\prod_{j=1}^{\nu}(a_j+i\,(x_j-b))\Big]\Big[\prod_{\ell=\nu}^{n}(a_\ell+i\,x_\ell)\Big]}\,,\end{aligned} \tag{5.255}$$

which we derived by induction. Here x_ℓ, a_ℓ and b are all real with $a_\ell\neq 0$. If we expand $\Big[\prod_{\ell=1}^{n_1-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)\Big]^{-1}$ in (5.254) as in (5.255), taking $b=\overline{k}_{n-n_1}$, we obtain:

$$\begin{aligned}\widetilde{G}_c^{(n,2)}(k_1,\ldots,k_n)=\mathfrak{R}(k_1,\ldots,k_n)-\sum_{n_1=2}^{n-2}\sum_{\nu=1}^{n_1-1}\Big[\prod_{\substack{\ell=1\\ \ell\neq n_1}}^{n-1}\sum_{\mathfrak{m}_\ell=1}^{\infty}\Big]\\ \times\frac{\triangle^{(n_1)}(\mathfrak{m}_1,\ldots,\mathfrak{m}_{n_1-1})\,\triangle^{(n-n_1)}(\mathfrak{m}_{n_1+1},\ldots,\mathfrak{m}_{n-1})}{\prod_{j=1}^{\nu}\left(E_{\mathfrak{m}_j}+i\,(\overline{k}_{n-j}-\overline{k}_{n-n_1})\right)\prod_{\substack{\ell=\nu\\ \ell\neq n_1}}^{n-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)}\,,\end{aligned} \tag{5.256}$$

where $\mathfrak{R}(k_1,\ldots,k_n)$ is given by:

$$\mathfrak{R}(k_1,\ldots,k_n) = -i\sum_{n_1=2}^{n-2}\Big[\prod_{\ell=1}^{n_1-1}\sum_{\mathfrak{m}_\ell=1}^{\infty}\Big]\Big[\prod_{\ell'=n_1+1}^{n-1}\sum_{\mathfrak{m}_{\ell'}=1}^{\infty}\Big]$$
$$\times\ \frac{\triangle^{(n_1)}(\mathfrak{m}_1,\ldots,\mathfrak{m}_{n_1-1})\,\triangle^{(n-n_1)}(\mathfrak{m}_{n_1+1},\ldots,\mathfrak{m}_{n-1})}{\prod_{\ell=1}^{n_1-1}\big(E_{\mathfrak{m}_\ell}+i\,(\overline{k}_{n-\ell}-\overline{k}_{n-n_1})\big)\prod_{\ell'=n_1+1}^{n-1}\big(E_{\mathfrak{m}_{\ell'}}+i\,\overline{k}_{n-\ell'}\big)}\,\mathrm{P}\Big(\frac{1}{\overline{k}_{n-n_1}}\Big)\,. \tag{5.257}$$

In deriving (5.256), we have used the fact that $\overline{k}_{n-n_1}\,\mathrm{P}\big(\frac{1}{\overline{k}_{n-n_1}}\big) = 1$. Now we shall show that the contribution of $\mathfrak{R}(k_1,\ldots,k_n)$ to $\overline{\mathsf{W}}_0^{(n,2)}[\widetilde{\varphi}]$ is actually zero, which implies the omission of $\mathfrak{R}(k_1,\ldots,k_n)$ from (5.256). Since $\overline{k}_{n-\ell}-\overline{k}_{n-n_1} = \sum_{j=1}^{n_1-\ell}k_{n-n_1+j}$ and $\prod_{\ell'=n_1+1}^{n-1}\big(E_{\mathfrak{m}_{\ell'}}+i\,\overline{k}_{n-\ell'}\big) = \prod_{\ell'=1}^{n-n_1-1}\big(E_{\mathfrak{m}_{n_1+\ell'}}+i\,\overline{k}_{n-n_1-\ell'}\big)$, it follows from (5.229) that:

$$\mathfrak{R}(k_1,\ldots,k_n) = -i\sum_{n_1=2}^{n-2}\widetilde{\mathfrak{J}}_d^{(n-n_1,1)}(k_1,\ldots,k_{n-n_1})$$
$$\times\ \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_{n-n_1+1},\ldots,k_n)\,\mathrm{P}\Big(\frac{1}{\overline{k}_{n-n_1}}\Big)\,. \tag{5.258}$$

If we make use of the fact that $\overline{k}_{n-n_1} = -\sum_{j=1}^{n_1}k_{n-n_1+j}$, which follows from $\overline{k}_n = 0$, and write $\mathrm{P}\big(\frac{1}{\overline{k}_{n-n_1}}\big) = -\mathrm{P}\big(1/\sum_{j=1}^{n_1}k_{n-n_1+j}\big)$, and then let $n_1 \to n-n_1$ in (5.258) we obtain:

$$\mathfrak{R}(k_1,\ldots,k_n) = i\sum_{n_1=2}^{n-2}\widetilde{\mathfrak{J}}_d^{(n-n_1,1)}(k_{n_1+1},\ldots,k_n)$$
$$\times\ \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,\ldots,k_{n_1})\,\mathrm{P}\Big(\frac{1}{\sum_{j=1}^{n-n_1}k_{n_1+j}}\Big)\,. \tag{5.259}$$

If we rename the k's in (5.259) such that:

$$\{k_1,k_2,\ldots,k_{n_1}\} \to \{k_{n-n_1+1},k_{n-n_1+2},\ldots,k_n\}\,,$$
$$\{k_{n_1+1},k_{n_1+2},\ldots,k_n\} \to \{k_1,k_2,\ldots,k_{n-n_1}\}\,, \tag{5.260}$$

we find that:

$$\mathfrak{R}(k_1,\ldots,k_{n-n_1},k_{n-n_1+1},\ldots,k_n) = -\,\mathfrak{R}(k_{n-n_1+1},\ldots,k_n,k_1,\ldots,k_{n-n_1})\,. \tag{5.261}$$

This leads to:

$$2\pi \int_{\mathbb{R}} \Big[\prod_{i=1}^{n} \frac{dk_i}{2\pi}\, \widetilde{\varphi}(k_i)\Big]\, \mathfrak{R}(k_1,\dots,k_n)\, \delta(k_1+\cdots+k_n) = 0\,, \tag{5.262}$$

which is the actual contribution of $\mathfrak{R}(k_1,\dots,k_n)$ to $\overline{\mathsf{W}}_0^{(n,2)}[\widetilde{\varphi}]$ as can be seen from (5.243) and (5.256). Hence, we can safely omit $\mathfrak{R}(k_1,\dots,k_n)$ from (5.256) and write:

$$\begin{aligned}\widetilde{G}_c^{(n,2)}(k_1,\dots,k_n) = &- \sum_{n_1=2}^{n-2} \sum_{\nu=1}^{n_1-1} \Big[\prod_{\substack{\ell=1\\ \ell\neq n_1}}^{n-1} \sum_{\mathsf{m}_\ell=1}^{\infty}\Big] \\ &\times \frac{\triangle^{(n_1)}(\mathsf{m}_1,\dots,\mathsf{m}_{n_1-1})\, \triangle^{(n-n_1)}(\mathsf{m}_{n_1+1},\dots,\mathsf{m}_{n-1})}{\prod_{j=1}^{\nu}\big(E_{\mathsf{m}_j} + i\,(\overline{k}_{n-j} - \overline{k}_{n-n_1})\big) \prod_{\substack{\ell=\nu\\ \ell\neq n_1}}^{n-1}\big(E_{\mathsf{m}_\ell} + i\,\overline{k}_{n-\ell}\big)}\,.\end{aligned} \tag{5.263}$$

This has a Taylor expansion around the origin $(k_1,\dots,k_n) = (0,\dots,0)$, allowing $\mathsf{W}_0^{(n,2)}[\varphi] = \overline{\mathsf{W}}_0^{(n,2)}[\widetilde{\varphi}]$ to have a local expansion for any field $\widetilde{\varphi}(k)$ with a compact support of a sufficiently small size interval.

Now we shall extend the above calculation to include $\widetilde{G}_c^{(n,3)}(k_1,\dots,k_n)$, showing that it can be Taylor expanded around the origin which supports the idea of $\mathsf{W}_0[\varphi]$ having a local expansion as in (5.191).

By using (5.234) in (5.240) and then comparing with (5.243) for $r=2$, we deduce that:

$$\begin{aligned}\widetilde{G}_c^{(n,3)}(k_1,..,k_n) = &\,\widetilde{\mathfrak{J}}_d^{(n,3)}(k_1,..,k_n) - 2\pi \sum_{n_1=2}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,..,k_{n_1})\, \widetilde{\mathfrak{J}}_d^{(n-n_1,2)}(k_{n_1+1},..,k_n) \\ &\times \delta(k_1+..+k_{n_1}) + \frac{4\pi^2}{3} \sum_{n_1=2}^{n-4} \sum_{n_2=2}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,..,k_{n_1})\, \widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_1+1},..,k_{n_1+n_2}) \\ &\times \widetilde{\mathfrak{J}}_d^{(n-n_1-n_2,1)}(k_{n_1+n_2+1},..,k_n)\, \delta(k_1+..+k_{n_1})\delta(k_{n_1+1}+..+k_{n_1+n_2})\,.\end{aligned} \tag{5.264}$$

To prove the existence of a local expansion of the functional $\mathsf{W}_0^{(n,3)}[\varphi]$ associated with $\widetilde{G}_c^{(n,3)}(k_1,\dots,k_n)$, we need to show first that all terms with Dirac δ-functions in (5.264)

do cancel. To do this let us start with expression (5.231) for $r = 3$, which reads as:

$$\widetilde{\mathfrak{J}}_d^{(n,3)}(k_1,\ldots,k_n) = \sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4} \sum_{\{\widetilde{\mathsf{m}}_1\}} \sum_{\{\widetilde{\mathsf{m}}_2\}} \sum_{\{\widetilde{\mathsf{m}}_3\}} \triangle^{(n_1)}(\widetilde{\mathsf{m}}_1)\,\triangle^{(n_2)}(\widetilde{\mathsf{m}}_2)\,\triangle^{(n_3)}(\widetilde{\mathsf{m}}_3) \times \frac{1}{\Big[\prod_{j=1}^{2}\big(\epsilon_j + i\,\overline{k}_{n-\overline{n}_j}\big)\Big]\Big[\prod\limits_{\substack{\ell=1\\ \ell\notin\{\overline{n}_1,\overline{n}_2\}}}^{n-1}\big(E_{\mathsf{m}_\ell} + i\,\overline{k}_{n-\ell}\big)\Big]}, \tag{5.265}$$

Employing (5.248) in (5.265) yields:

$$\widetilde{\mathfrak{J}}_d^{(n,3)}(k_1,\ldots,k_n) = \sum_{i=1}^{4} \Upsilon_i(k_1,\ldots,k_n)\,, \tag{5.266}$$

where

$$\Upsilon_1(k_1,..,k_n) = \pi^2 \sum_{n_1=2}^{n-4}\sum_{n_2=2}^{n-4} \mathfrak{S}^{(n_1,n_2)}(k_1,..,k_n)\,\delta(\overline{k}_{n-n_1})\,\delta(\overline{k}_{n-n_1-n_2}), \tag{5.267}$$

$$\Upsilon_2(k_1,..,k_n) = -i\pi \sum_{n_1=2}^{n-4}\sum_{n_2=2}^{n-4} \mathfrak{S}^{(n_1,n_2)}(k_1,..,k_n)\,\delta(\overline{k}_{n-n_1})\,\mathrm{P}\left(\frac{1}{\overline{k}_{n-n_1-n_2}}\right), \tag{5.268}$$

$$\Upsilon_3(k_1,..,k_n) = -i\pi \sum_{n_1=2}^{n-4}\sum_{n_2=2}^{n-4} \mathfrak{S}^{(n_1,n_2)}(k_1,..,k_n)\,\delta(\overline{k}_{n-n_1-n_2})\,\mathrm{P}\left(\frac{1}{\overline{k}_{n-n_1}}\right), \tag{5.269}$$

$$\Upsilon_4(k_1,..,k_n) = -\sum_{n_1=2}^{n-4}\sum_{n_2=2}^{n-4} \mathfrak{S}^{(n_1,n_2)}(k_1,..,k_n)\,\mathrm{P}\left(\frac{1}{\overline{k}_{n-n_1}}\right)\mathrm{P}\left(\frac{1}{\overline{k}_{n-n_1-n_2}}\right), \tag{5.270}$$

with $\mathfrak{S}^{(n_1,n_2)}(k_1,..,k_n)$ defined as:

$$\mathfrak{S}^{(n_1,n_2)}(k_1,..,k_n) = \Big[\prod_{\substack{\ell=1\\ \ell\notin\{n_1,n_1+n_2\}}}^{n-1}\Big] \sum_{\mathsf{m}_\ell=1}^{\infty} \frac{\triangle^{(n_1)}(\mathsf{m}_1,..,\mathsf{m}_{n_1-1})}{\prod_{\ell=1}^{n_1-1}\big(E_{\mathsf{m}_\ell} + i\,\overline{k}_{n-\ell}\big)} \frac{\triangle^{(n_2)}(\mathsf{m}_{n_1+1},..,\mathsf{m}_{n_1+n_2-1})}{\prod_{\ell'=n_1+1}^{n_1+n_2-1}\big(E_{\mathsf{m}_{\ell'}} + i\,\overline{k}_{n-\ell'}\big)} \times \frac{\triangle^{(n-n_1-n_2)}(\mathsf{m}_{n_1+n_2+1},..,\mathsf{m}_{n-1})}{\prod_{\ell''=n_1+n_2+1}^{n-1}\big(E_{\mathsf{m}_{\ell''}} + i\,\overline{k}_{n-\ell''}\big)}. \tag{5.271}$$

Now, we shall consider each term $\Upsilon_i(k_1,..,k_n)$ in (5.266) separately. Beginning with (5.267), we note that due to the δ-function constraints $\delta(\overline{k}_{n-n_1})$ and $\delta(\overline{k}_{n-n_1-n_2})$ in this

expression of $\Upsilon_1(k_1,..,k_n)$ we can write:

$$\prod_{\ell=1}^{n_1-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)=\prod_{\ell=1}^{n_1-1}\left(E_{\mathfrak{m}_\ell}+i\sum_{j=1}^{n_1-\ell}k_{n-n_1+j}\right), \tag{5.272}$$

$$\prod_{\ell'=n_1+1}^{n_1+n_2-1}\left(E_{\mathfrak{m}_{\ell'}}+i\,\overline{k}_{n-\ell'}\right)=\prod_{\ell'=1}^{n_2-1}\left(E_{\mathfrak{m}_{n_1+\ell'}}+i\sum_{j=1}^{n_2-\ell'}k_{n-n_1-n_2+j}\right), \tag{5.273}$$

$$\prod_{\ell''=n_1+n_2+1}^{n-1}\left(E_{\mathfrak{m}_{\ell''}}+i\,\overline{k}_{n-\ell''}\right)=\prod_{\ell''=1}^{n-n_1-n_2-1}\left(E_{\mathfrak{m}_{n_1+n_2+\ell''}}+i\sum_{j=1}^{n-n_1-n_2-\ell''}k_j\right). \tag{5.274}$$

Also, we can show that:

$$\delta(\overline{k}_{n-n_1})\,\delta(\overline{k}_{n-n_1-n_2})=\delta\Big(\sum_{j=1}^{n_2}k_{n-n_1-n_2+j}\Big)\,\delta(\overline{k}_{n-n_1-n_2})\,. \tag{5.275}$$

From (5.272)–(5.275), it follows that:

$$\begin{aligned}\Upsilon_1(k_1,..,k_n)=\pi^2\sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4}&\Big[\prod_{\substack{\ell=1\\ \ell\notin\{n_1,n_1+n_2\}}}^{n-1}\sum_{\mathfrak{m}_\ell=1}^{\infty}\Big]\frac{\triangle^{(n_1)}(\mathfrak{m}_1,..,\mathfrak{m}_{n_1-1})}{\prod_{\ell=1}^{n_1-1}\Big(E_{\mathfrak{m}_\ell}+i\sum_{j=1}^{n_1-\ell}k_{n_2+n_3+j}\Big)}\\ &\times\frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1},..,\mathfrak{m}_{n_1+n_2-1})}{\prod_{\ell'=1}^{n_2-1}\Big(E_{\mathfrak{m}_{n_1+\ell'}}+i\sum_{j=1}^{n_2-\ell'}k_{n_3+j}\Big)}\;\frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1},..,\mathfrak{m}_{n-1})}{\prod_{\ell''=1}^{n_3-1}\Big(E_{\mathfrak{m}_{n_1+n_2+\ell''}}+i\sum_{j=1}^{n_3-\ell''}k_j\Big)}\\ &\times\delta\Big(\sum_{j=1}^{n_2}k_{n_3+j}\Big)\,\delta(\overline{k}_{n_3})\,.\end{aligned} \tag{5.276}$$

By making use of (5.229) in (5.276), we obtain:

$$\begin{aligned}\Upsilon_1(k_1,..,k_n)=\pi^2\sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4}&\widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_{n_2+n_3+1},..,k_n)\,\widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_3+1},..,k_{n_3+n_2})\\ &\times\widetilde{\mathfrak{J}}_d^{(n_3,1)}(k_1,..,k_{n_3})\,\delta(k_1+..+k_{n_3})\,\delta(k_{n_3+1}+..+k_{n_3+n_2})\,,\end{aligned} \tag{5.277}$$

which by interchanging n_1 with n_3 we can rewrite as:

$$\Upsilon_1(k_1,..,k_n) = \pi^2 \sum_{n_1=2}^{n-4} \sum_{n_2=2}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,..,k_{n_1})\, \widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_1+1},..,k_{n_1+n_2}) \times \widetilde{\mathfrak{J}}_d^{(n-n_1-n_2,1)}(k_{n_1+n_2+1},..,k_n)\, \delta(k_1+..+k_{n_1})\, \delta(k_{n_1+1}+..+k_{n_1+n_2})\,. \tag{5.278}$$

This has the same form as the third term in (5.264).

Now, let us consider $\Upsilon_2(k_1,..,k_n)$ in (5.268) which we can rewrite as:

$$\Upsilon_2(k_1,..,k_n) = -i\pi \sum_{\substack{n_1,n_2,n_3=2 \\ n_1+n_2+n_3=n}}^{n-4} \Big[\prod_{\ell\notin\{n_1,n_1+n_2\}}^{n-1} \sum_{\mathfrak{m}_\ell=1}^{\infty} \Big] \frac{\triangle^{(n_1)}(\mathfrak{m}_1,..,\mathfrak{m}_{n_1-1})}{\prod_{\ell=1}^{n_1-1} \Big(E_{\mathfrak{m}_\ell} + i \sum_{j=1}^{n_1-\ell} k_{n_2+n_3+j}\Big)} \times \frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1},..,\mathfrak{m}_{n_1+n_2-1})}{\prod_{\ell'=1}^{n_2-1} \Big(E_{\mathfrak{m}_{n_1+\ell'}} + i\,\overline{k}_{n_2+n_3-\ell'}\Big)} \frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1},..,\mathfrak{m}_{n-1})}{\prod_{\ell''=n_1+n_2+1}^{n-1} \Big(E_{\mathfrak{m}_{\ell''}} + i\,\overline{k}_{n-\ell''}\Big)} \times \delta(\overline{k}_{n_2+n_3})\, \mathrm{P}\Big(\frac{1}{\overline{k}_{n_3}}\Big)\,. \tag{5.279}$$

By making use of (5.229) and employing (5.255), with the free parameter b taken as $\overline{k}_{n_3}$, to expand $\Big[\prod_{\ell'=1}^{n_2-1} \big(E_{\mathfrak{m}_{n_1+\ell'}} + i\,\overline{k}_{n_2+n_3-\ell'}\big)\Big]^{-1}$ in (5.279) we obtain:

$$\Upsilon_2(k_1,...,k_n) = \mathcal{A}(k_1,...,k_n) + \mathcal{B}(k_1,...,k_n)\,, \tag{5.280}$$

where

$$\mathcal{A}(k_1,...,k_n) = -i\pi \sum_{\substack{n_1,n_2,n_3=2 \\ n_1+n_2+n_3=n}}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_{n_2+n_3+1},...,k_n) \Big[\prod_{\substack{\ell=n_1+1 \\ \ell\neq n_1+n_2}}^{n-1} \sum_{\mathfrak{m}_\ell=1}^{\infty} \Big] \times \frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1},..,\mathfrak{m}_{n_1+n_2-1})}{\prod_{\ell'=1}^{n_2-1} \Big(E_{\mathfrak{m}_{n_1+\ell'}} + i\,(\overline{k}_{n_2+n_3-\ell'} - \overline{k}_{n_3})\Big)} \frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1},..,\mathfrak{m}_{n-1})}{\prod_{\ell''=n_1+n_2+1}^{n-1} \Big(E_{\mathfrak{m}_{\ell''}} + i\,\overline{k}_{n-\ell''}\Big)} \times \delta(\overline{k}_{n_2+n_3})\, \mathrm{P}\Big(\frac{1}{\overline{k}_{n_3}}\Big)\,, \tag{5.281}$$

and

$$\mathcal{B}(k_1,...,k_n) = -\pi \sum_{n_1=2}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_{n-n_1+1},...,k_n) \sum_{n_2=2}^{n-4} \sum_{\nu=1}^{n_2-1} \Big[\prod_{\substack{\ell=n_1+1 \\ \ell\neq n_1+n_2}}^{n-1} \sum_{\mathfrak{m}_\ell=1}^{\infty} \Big]$$
$$\times \frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1},..,\mathfrak{m}_{n_1+n_2-1})}{\prod_{j=1}^{\nu}\Big(E_{\mathfrak{m}_{n_1+j}} + i\,(\overline{k}_{n-n_1-j} - \overline{k}_{n-n_1-n_2})\Big)} \frac{\triangle^{(n-n_1-n_2)}(\mathfrak{m}_{n_1+n_2+1},..,\mathfrak{m}_{n-1})}{\prod_{\substack{\ell=\nu \\ \ell\neq n_2}}^{n-n_1-1}\Big(E_{\mathfrak{m}_{n_1+\ell}} + i\,\overline{k}_{n-n_1-\ell}\Big)}$$
$$\times\ \delta(\overline{k}_{n-n_1})\,. \tag{5.282}$$

Using (5.274) in (5.281) together with the fact that $\overline{k}_{n_2+n_3-\ell'} - \overline{k}_{n_3} = \sum_{j=1}^{n_2-\ell'} k_{n_3+j}$ allows us with the help of (5.229) to express $\mathcal{A}(k_1,...,k_n)$ as:

$$\mathcal{A}(k_1,...,k_n) = -i\,\pi \sum_{n_1=2}^{n-4} \sum_{n_2=2}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,..,k_{n_1})\, \widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_1+1},..,k_{n_1+n_2})$$
$$\times\, \widetilde{\mathfrak{J}}_d^{(n-n_1-n_2,1)}(k_{n_1+n_2+1},..,k_n)\, \delta(k_1+..+k_{n_1+n_2})\, \mathrm{P}\left(\frac{1}{k_1+..+k_{n_1}}\right). \tag{5.283}$$

If we replace $\delta(k_1 + ... + k_{n_1+n_2})\,\mathrm{P}\left(\frac{1}{k_1+...+k_{n_1}}\right)$ in (5.283) by its equivalence $-\,\delta(k_1+..+k_{n_1+n_2})\,\mathrm{P}\left(\frac{1}{k_{n_1}+...+k_{n_1+n_2}}\right)$ and then rename the relevant k's such that:

$$\{k_1,k_2,\ldots,k_{n_1}\} \to \{k_{n_2+1},k_{n_2+2},\ldots,k_{n_2+n_1}\}\,,$$
$$\{k_{n_1+1},k_{n_1+2},\ldots,k_{n_1+n_2}\} \to \{k_1,k_2,\ldots,k_{n_2}\}\,, \tag{5.284}$$

we find, after interchanging n_1 with n_2, that $\mathcal{A}(k_1,\ldots,k_n) \to -\,\mathcal{A}(k_1,\ldots,k_n)$ in the integration $\int_{\mathbb{R}} \Big[\prod_{i=1}^{n} \frac{dk_i}{2\pi}\,\widetilde{\varphi}(k_i)\Big]\,\mathcal{A}(k_1,\ldots,k_n)\,\delta(\overline{k}_n)$, giving the integral as minus itself. This implies that $\mathcal{A}(k_1,\ldots,k_n)$, as it appears in the integrand of (5.243) via $\widetilde{G}_c^{(n,r)}(k_1,\ldots,k_n)$ for $r=3$, yields a zero contribution to $\overline{\mathsf{W}}_0^{(n,3)}[\widetilde{\varphi}]$. Hence, we can safely omit $\mathcal{A}(k_1,\ldots,k_n)$ from (5.280).

It follows from (5.227) that $\triangle^{(n-n_1-n_2)}(\mathfrak{m}_{n_1+n_2+1},\ldots,\mathfrak{m}_{n-1}) = 0$ for all $n_2 > n-n_1-2$. This truncates the sum $\sum_{n_2=2}^{n-4}$ in (5.282) at $n_2 = n-n_1-2$, allow-

ing us to use (5.263) for expressing $\mathcal{B}(k_1,\ldots,k_n)$ as:

$$\mathcal{B}(k_1,..,k_n) = \pi \sum_{n_1=2}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_{n-n_1+1},..,k_n)\, \widetilde{G}_c^{(n-n_1,2)}(k_1,..,k_{n-n_1})\, \delta(\overline{k}_{n-n_1})\,. \tag{5.285}$$

Being a term in $\widetilde{G}_c^{(n,3)}(k_1,\ldots,k_n)$, $\mathcal{B}(k_1,\ldots,k_n)$ will always appear in the integrand of (5.243) multiplied by a product of functions $\widetilde{\varphi}(k_1)\ldots\widetilde{\varphi}(k_n)\,\delta(\overline{k}_n)$, which is symmetric in the k-variables. Hence, we can safely rename the arguments of the Green's functions in (5.285), rewriting $\mathcal{B}(k_1,\ldots,k_n)$ as:

$$\mathcal{B}(k_1,...,k_n) = \pi \sum_{n_1=2}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,...,k_{n_1})\, \widetilde{G}_c^{(n-n_1,2)}(k_{n_1+1},...,k_n)\, \delta(k_1+\cdots+k_{n_1}). \tag{5.286}$$

By substituting (5.247) for $\widetilde{G}_c^{(n-n_1,2)}(k_{n_1+1},...,k_n)$ in (5.286), we obtain:

$$\begin{aligned}
\mathcal{B}(k_1,...,k_n) &= \pi \sum_{n_1=2}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,...,k_{n_1})\, \widetilde{\mathfrak{J}}_d^{(n-n_1,2)}(k_{n_1+1},...,k_n)\, \delta(k_1+\cdots+k_{n_1}) \\
&\quad -\pi^2 \sum_{n_1=2}^{n-4}\sum_{n_2=2}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,...,k_{n_1})\, \widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_1+1},...,k_{n_1+n_2}) \\
&\quad \times \widetilde{\mathfrak{J}}_d^{(n-n_1-n_2,1)}(k_{n_1+n_2+1},...,k_n)\delta(k_1+...+k_{n_1})\delta(k_{n_1+1}+...+k_{n_1+n_2})\,, \\
&= \Upsilon_2(k_1,...,k_n)\,,
\end{aligned} \tag{5.287}$$

where the last result follows from (5.280) after omitting $\mathcal{A}(k_1,...,k_n)$. By repeating the same argument that led to (5.287) in (5.269) we can show that:

$$\Upsilon_3(k_1,\ldots,k_n) = -\mathcal{A}(k_1,...,k_n) + \mathcal{B}(k_1,\ldots,k_n)\,, \tag{5.288}$$

which, after omitting the first term, reduces to:

$$\Upsilon_3(k_1,\ldots,k_n) = \Upsilon_2(k_1,\ldots,k_n) = \mathcal{B}(k_1,\ldots,k_n)\,. \tag{5.289}$$

Now, we shall consider $\Upsilon_4(k_1,\ldots,k_n)$ in (5.270) which we rewrite here as:

$$\Upsilon_4(k_1,\ldots,k_n) = -\sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4}\Bigg[\prod_{\substack{\ell=1\\ \ell\notin\{n_1,n_1+n_2\}}}^{n-1}\sum_{\mathfrak{m}_\ell=1}^{\infty}\Bigg]\frac{\triangle^{(n_1)}(\mathfrak{m}_1,\ldots,\mathfrak{m}_{n_1-1})}{\prod_{\ell=1}^{n_1-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)}$$
$$\times\frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1},\ldots,\mathfrak{m}_{n_1+n_2-1})}{\prod_{\ell'=1}^{n_2-1}\left(E_{\mathfrak{m}_{n_1+\ell'}}+i\,\overline{k}_{n_2+n_3-\ell'}\right)}\frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1},\ldots,\mathfrak{m}_{n-1})}{\prod_{\ell''=n_1+n_2+1}^{n-1}\left(E_{\mathfrak{m}_{\ell''}}+i\,\overline{k}_{n-\ell''}\right)}$$
$$\times\,\mathrm{P}\left(\frac{1}{\overline{k}_{n_2+n_3}}\right)\mathrm{P}\left(\frac{1}{\overline{k}_{n_3}}\right). \tag{5.290}$$

By expanding $\left[\prod_{\ell=1}^{n_1-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)\right]^{-1}$ and $\left[\prod_{\ell'=1}^{n_2-1}\left(E_{\mathfrak{m}_{n_1+\ell'}}+i\,\overline{k}_{n_2+n_3-\ell'}\right)\right]^{-1}$ in (5.290) according to (5.255), taking the free parameter b in each case as $\overline{k}_{n_2+n_3}$ and $\overline{k}_{n_3}$ respectively, we obtain:

$$\Upsilon_4(k_1,..,k_n) = \sum_{i=1}^{3}\Lambda_i(k_1,..,k_n) + \sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4}\Bigg[\prod_{\substack{\ell=1\\ \ell\notin\{n_1,n_1+n_2\}}}^{n-1}\sum_{\mathfrak{m}_\ell=1}^{\infty}\Bigg]\frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1},..,\mathfrak{m}_{n-1})}{\prod_{\ell=n_1+n_2+1}^{n-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)}$$
$$\times\sum_{\nu=1}^{n_1-1}\frac{\triangle^{(n_1)}(\mathfrak{m}_1,\ldots,\mathfrak{m}_{n_1-1})}{\prod_{j=1}^{\nu}\left(E_{\mathfrak{m}_j}+i\left(\overline{k}_{n-j}-\overline{k}_{n-n_1}\right)\right)\prod_{\ell=\nu}^{n_1-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)}$$
$$\times\sum_{\nu'=1}^{n_2-1}\frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1},\ldots,\mathfrak{m}_{n_1+n_2-1})}{\prod_{j=n_1+1}^{n_1+\nu'}\left(E_{\mathfrak{m}_j}+i\left(\overline{k}_{n-j}-\overline{k}_{n_3}\right)\right)\prod_{\ell=n_1+\nu'}^{n_1+n_2-1}\left(E_{\mathfrak{m}_\ell}+i\,\overline{k}_{n-\ell}\right)}, \tag{5.291}$$

where

$$\Lambda_1(k_1,\ldots,k_n) = -\sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4}\Bigg[\prod_{\substack{\ell=1\\ \ell\notin\{n_1,n_1+n_2\}}}^{n-1}\sum_{\mathfrak{m}_\ell=1}^{\infty}\Bigg]\frac{\triangle^{(n_1)}(\mathfrak{m}_1,\ldots,\mathfrak{m}_{n_1-1})}{\prod_{\ell=1}^{n_1-1}\left(E_{\mathfrak{m}_\ell}+i\left(\overline{k}_{n-\ell}-\overline{k}_{n-n_1}\right)\right)}$$
$$\times\frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1},\ldots,\mathfrak{m}_{n_1+n_2-1})}{\prod_{\ell'=1}^{n_2-1}\left(E_{\mathfrak{m}_{n_1+\ell'}}+i\left(\overline{k}_{n_2+n_3-\ell'}-\overline{k}_{n_3}\right)\right)}\frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1},\ldots,\mathfrak{m}_{n-1})}{\prod_{\ell''=n_1+n_2+1}^{n-1}\left(E_{\mathfrak{m}_{\ell''}}+i\,\overline{k}_{n-\ell''}\right)}$$
$$\times\,\mathrm{P}\left(\frac{1}{\overline{k}_{n_2+n_3}}\right)\mathrm{P}\left(\frac{1}{\overline{k}_{n_3}}\right), \tag{5.292}$$

$$\Lambda_2(k_1,\ldots,k_n) = i \sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4} \Bigg[\prod_{\substack{\ell=1\\ \ell\notin\{n_1,n_1+n_2\}}}^{n-1} \sum_{\mathfrak{m}_\ell=1}^{\infty} \Bigg] \frac{\triangle^{(n_1)}(\mathfrak{m}_1,\ldots,\mathfrak{m}_{n_1-1})}{\prod_{\ell=1}^{n_1-1}\Big(E_{\mathfrak{m}_\ell} + i\left(\overline{k}_{n-\ell} - \overline{k}_{n-n_1}\right)\Big)}$$
$$\times \sum_{\nu=1}^{n_2-1} \frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1},\ldots,\mathfrak{m}_{n_1+n_2-1})}{\prod_{j=1}^{\nu}\Big(E_{\mathfrak{m}_{n_1+j}} + i\left(\overline{k}_{n_2+n_3-j} - \overline{k}_{n_3}\right)\Big) \prod_{\ell=\nu}^{n_2-1}\Big(E_{\mathfrak{m}_{n_1+\ell}} + i\,\overline{k}_{n_2+n_3-\ell}\Big)}$$
$$\times \frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1},\ldots,\mathfrak{m}_{n-1})}{\prod_{\ell'=n_1+n_2+1}^{n-1}\Big(E_{\mathfrak{m}_{\ell'}} + i\,\overline{k}_{n-\ell'}\Big)} \; \mathrm{P}\left(\frac{1}{\overline{k}_{n_2+n_3}}\right), \tag{5.293}$$

and

$$\Lambda_3(k_1,\ldots,k_n) = i \sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4} \Bigg[\prod_{\substack{\ell=1\\ \ell\notin\{n_1,n_1+n_2\}}}^{n-1} \sum_{\mathfrak{m}_\ell=1}^{\infty} \Bigg] \frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1},\ldots,\mathfrak{m}_{n_1+n_2-1})}{\prod_{\ell=1}^{n_2-1}\Big(E_{\mathfrak{m}_{n_1+\ell}} + i\left(\overline{k}_{n_2+n_3-\ell} - \overline{k}_{n_3}\right)\Big)}$$
$$\times \sum_{\nu=1}^{n_1-1} \frac{\triangle^{(n_1)}(\mathfrak{m}_1,\ldots,\mathfrak{m}_{n_1-1})}{\prod_{j=1}^{\nu}\Big(E_{\mathfrak{m}_j} + i\left(\overline{k}_{n-j} - \overline{k}_{n-n_1}\right)\Big) \prod_{\ell=\nu}^{n_1-1}\Big(E_{\mathfrak{m}_\ell} + i\,\overline{k}_{n-\ell}\Big)}$$
$$\times \frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1},\ldots,\mathfrak{m}_{n-1})}{\prod_{\ell'=n_1+n_2+1}^{n-1}\Big(E_{\mathfrak{m}_{\ell'}} + i\,\overline{k}_{n-\ell'}\Big)} \; \mathrm{P}\left(\frac{1}{\overline{k}_{n_3}}\right). \tag{5.294}$$

Now, we shall show how the principal value distributions in each Λ_i cancel in the integration of (5.243) where they appear as terms of $\widetilde{G}_c^{(n,3)}(k_1,\ldots,k_n)$. Starting with expression (5.292) and making use of (5.229) allows us to rewrite $\Lambda_1(k_1,\ldots,k_n)$ as:

$$\Lambda_1 = -\sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,\ldots,k_{n_1})\,\widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_1+1},\ldots,k_{n_1+n_2})\,\widetilde{\mathfrak{J}}_d^{(n_3,1)}(k_{n_1+n_2+1},\ldots,k_n)$$
$$\times \quad \mathrm{P}\left(\frac{1}{\overline{k}_{n_1+n_2}}\right)\mathrm{P}\left(\frac{1}{\overline{k}_{n_1}}\right). \tag{5.295}$$

If we rename the arguments of $\widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,\ldots,k_{n_1})$ and $\widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_1+1},\ldots,k_{n_1+n_2})$ in (5.295)

according to:

$$\{k_1, k_2, \ldots, k_{n_1}\} \to \{k'_1, k'_2, \ldots, k'_{n_1}\} = \{k_{n_2+1}, k_{n_2+2}, \ldots, k_{n_2+n_1}\},$$
$$\{k_{n_1+1}, k_{n_1+2}, \ldots, k_{n_1+n_2}\} \to \{k''_1, k''_2, \ldots, k''_{n_2}\} = \{k_1, k_2, \ldots, k_{n_2}\}, \tag{5.296}$$

and then interchange n_1 with n_2, we obtain:

$$\Lambda_1 = -\sum_{\substack{n_1,n_2,n_3=2 \\ n_1+n_2+n_3=n}}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1, ..., k_{n_1})\, \widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_1+1}, ..., k_{n_1+n_2})\, \widetilde{\mathfrak{J}}_d^{(n_3,1)}(k_{n_1+n_2+1}, ..., k_n)$$
$$\times \quad \mathrm{P}\left(\frac{1}{\overline{k}_{n_1+n_2}}\right) \mathrm{P}\left(\frac{1}{\overline{k}_{n_1+n_2} - \overline{k}_{n_1}}\right). \tag{5.297}$$

Also, if we use the fact that $\overline{k}_{n_1+n_2} = -\sum_{j=1}^{n_3} k_{n_1+n_2+j}$ in (5.295) and rename the k's according to:

$$\{k_1, k_2, \ldots, k_{n_1}\} \to \{k'_1, k'_2, \ldots, k'_{n_1}\} = \{k_{n_3+1}, k_{n_3+2}, \ldots, k_{n_3+n_1}\},$$
$$\{k_{n_1+1}, k_{n_1+2}, \ldots, k_{n_1+n_2}\} \to \{k''_1, k''_2, \ldots, k''_{n_2}\} = \{k_{n_3+n_1+1}, k_{n_3+n_1+2}, \ldots, k_n\},$$
$$\{k_{n_1+n_2+1}, k_{n_1+n_2+2}, \ldots, k_n\} \to \{k'''_1, k'''_2, \ldots, k'''_{n_3}\} = \{k_1, k_2, \ldots, k_{n_3}\}, \tag{5.298}$$

we find, after interchanging n_1 with n_3 first and n_2 with n_3 next, that:

$$\Lambda_1 = \sum_{\substack{n_1,n_2,n_3=2 \\ n_1+n_2+n_3=n}}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1, ..., k_{n_1})\, \widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_1+1}, ..., k_{n_1+n_2})\, \widetilde{\mathfrak{J}}_d^{(n_3,1)}(k_{n_1+n_2+1}, ..., k_n)$$
$$\times \quad \mathrm{P}\left(\frac{1}{\overline{k}_{n_1}}\right) \mathrm{P}\left(\frac{1}{\overline{k}_{n_1+n_2} - \overline{k}_{n_1}}\right). \tag{5.299}$$

In the integrand of (5.243), we can express $\Lambda_1(k_1, ..., k_n)$ as a sum of (5.295), (5.297) and (5.299) divided by 3 in which case we can use the following identity [63]:

$$\mathrm{P}\left(\frac{1}{x}\right) \mathrm{P}\left(\frac{1}{y}\right) + \mathrm{P}\left(\frac{1}{x-y}\right) \left[\mathrm{P}\left(\frac{1}{x}\right) - \mathrm{P}\left(\frac{1}{y}\right)\right] = \pi^2\, \delta(x)\, \delta(y), \tag{5.300}$$

to rewrite $\Lambda_1(k_1,...,k_n)$ in a form free of the principal value distributions, giving:

$$\Lambda_1(k_1,...,k_n) = -\frac{\pi^2}{3} \sum_{\substack{n_1,n_2,n_3=2 \\ n_1+n_2+n_3=n}}^{n-4} \widetilde{\mathfrak{J}}_d^{(n_1,1)}(k_1,...,k_{n_1})\, \widetilde{\mathfrak{J}}_d^{(n_2,1)}(k_{n_1+1},...,k_{n_1+n_2}) \times \widetilde{\mathfrak{J}}_d^{(n_3,1)}(k_{n_1+n_2+1},...,k_n)\, \delta(\overline{k}_{n_1})\, \delta(\overline{k}_{n_1+n_2})\,. \tag{5.301}$$

Having achieved this result, we shall now consider both $\Lambda_2(k_1,...,k_n)$ and $\Lambda_3(k_1,...,k_n)$, showing that their sum is independent of any principal value distribution. To prove this, let us first make use of (5.244) and (5.263) to rewrite $\Lambda_2(k_1,...,k_n)$ as:

$$\Lambda_2(k_1,..,k_n) = -i \sum_{n_1=2}^{n-4} \widetilde{G}_c^{(n-n_1,2)}(k_1,..,k_{n-n_1}) \widetilde{G}_c^{(n_1,1)}(k_{n-n_1+1},..,k_n)\, \mathrm{P}\left(\frac{1}{\overline{k}_{n-n_1}}\right). \tag{5.302}$$

Next, we consider (5.294), which can be used to show that $\Lambda_3(k_1,...,k_n)$ is composed of $-\Lambda_2(k_1,...,k_n)$ plus other additional terms free of the principal value distributions. By expanding $\left[\prod_{\ell=\nu}^{n_1-1}\left(E_{\mathrm{m}_\ell} + i\,\overline{k}_{n-\ell}\right)\right]^{-1}$ in (5.294) according to (5.255):

$$\frac{1}{\prod_{\ell=\nu}^{n_1-1}\left(E_{\mathrm{m}_\ell} + i\,\overline{k}_{n-\ell}\right)} = \frac{1}{\prod_{\ell=\nu}^{n_1-1}\left(E_{\mathrm{m}_\ell} + i\,(\overline{k}_{n-\ell} - \overline{k}_{n_3})\right)} - i\,\overline{k}_{n_3} \sum_{\gamma=\nu}^{n_1-1} \frac{1}{\prod_{j=\nu}^{\gamma}\left(E_{\mathrm{m}_j} + i\,(\overline{k}_{n-j} - \overline{k}_{n_3})\right) \prod_{\ell=\gamma}^{n_1-1}\left(E_{\mathrm{m}_\ell} + i\,\overline{k}_{n-\ell}\right)}, \tag{5.303}$$

and using the fact that $\prod_{\ell=1}^{n_2-1}\left(E_{\mathrm{m}_{n_1+\ell}} + i\,(\overline{k}_{n_2+n_3-\ell} - \overline{k}_{n_3})\right) = \prod_{\ell=n_1+1}^{n_1+n_2-1}\left(E_{\mathrm{m}_\ell} + i\,(\overline{k}_{n-\ell} - \overline{k}_{n_3})\right)$, we obtain:

$$\Lambda_3(k_1,..,k_n) = \Xi_1(k_1,..,k_n) + \Xi_2(k_1,..,k_n)\,, \tag{5.304}$$

where

$$\Xi_1(k_1,\ldots,k_n) = i \sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4} \sum_{\nu=1}^{n_1-1} \Bigg[\prod_{\substack{\ell=1\\ \ell\notin\{n_1,n_1+n_2\}}}^{n-1} \sum_{\mathrm{m}_\ell=1}^{\infty} \Bigg] \frac{\triangle^{(n_3)}(\mathrm{m}_{n_1+n_2+1},\ldots,\mathrm{m}_{n-1})}{\prod_{\ell'=n_1+n_2+1}^{n-1} \left(E_{\mathrm{m}_{\ell'}} + i\,\overline{k}_{n-\ell'}\right)}$$
$$\times \frac{\triangle^{(n_1)}(\mathrm{m}_1,\ldots,\mathrm{m}_{n_1-1})\ \triangle^{(n_2)}(\mathrm{m}_{n_1+1},\ldots,\mathrm{m}_{n_1+n_2-1})}{\prod_{j=1}^{\nu}\left(E_{\mathrm{m}_j} + i\left(\overline{k}_{n-j} - \overline{k}_{n-n_1}\right)\right) \prod_{\substack{\ell=\nu\\ \ell\neq n_1}}^{n_1+n_2-1}\left(E_{\mathrm{m}_\ell} + i\left(\overline{k}_{n-\ell} - \overline{k}_{n_3}\right)\right)} \mathrm{P}\left(\frac{1}{\overline{k}_{n_3}}\right), \quad (5.305)$$

and

$$\Xi_2(k_1,\ldots,k_n) = \sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4} \sum_{\nu=1}^{n_1-1} \sum_{\gamma=\nu}^{n_1-1} \Bigg[\prod_{\substack{\ell=1\\ \ell\notin\{n_1,n_1+n_2\}}}^{n-1} \sum_{\mathrm{m}_\ell=1}^{\infty} \Bigg]$$
$$\times \frac{\triangle^{(n_1)}(\mathrm{m}_1,\ldots,\mathrm{m}_{n_1-1})}{\prod_{j=1}^{\nu}\left(E_{\mathrm{m}_j} + i\left(\overline{k}_{n-j} - \overline{k}_{n-n_1}\right)\right) \prod_{\ell=\nu}^{\gamma}\left(E_{\mathrm{m}_\ell} + i\left(\overline{k}_{n-\ell} - \overline{k}_{n_3}\right)\right) \prod_{\ell'=\gamma}^{n_1-1}\left(E_{\mathrm{m}_{\ell'}} + i\,\overline{k}_{n-\ell'}\right)}$$
$$\times \frac{\triangle^{(n_2)}(\mathrm{m}_{n_1+1},\ldots,\mathrm{m}_{n_1+n_2-1})}{\prod_{\ell=n_1+1}^{n_1+n_2-1}\left(E_{\mathrm{m}_\ell} + i\left(\overline{k}_{n-\ell} - \overline{k}_{n_3}\right)\right)} \frac{\triangle^{(n_3)}(\mathrm{m}_{n_1+n_2+1},\ldots,\mathrm{m}_{n-1})}{\prod_{\ell'=n_1+n_2+1}^{n-1}\left(E_{\mathrm{m}_{\ell'}} + i\,\overline{k}_{n-\ell'}\right)}. \quad (5.306)$$

Now, if we rearrange the summations over the k's in (5.305) such that:

$$\overline{k}_{n-j} - \overline{k}_{n-n_1} = \sum_{r=1}^{n-n_3-j} k_{n_3+r} - \sum_{r=1}^{n-n_3-n_1} k_{n_3+r}\,, \qquad \overline{k}_{n-\ell} - \overline{k}_{n_3} = \sum_{r=1}^{n-n_3-\ell} k_{n_3+r}\,, \quad (5.307)$$

we can show from (5.244) and (5.263) that:

$$\Xi_1(k_1,..,k_n) = i \sum_{n_3=2}^{n-4} \widetilde{G}_c^{(n_3,1)}(k_1,..,k_{n_3})\widetilde{G}_c^{(n-n_3,2)}(k_{n_3+1},..,k_n)\,\mathrm{P}\left(\frac{1}{\sum_{r=1}^{n-n_3} k_{n_3+r}}\right). \quad (5.308)$$

Here, we have used the fact that $\overline{k}_{n_3} = -\sum_{r=1}^{n-n_3} k_{n_3+r}$, which follows from the constraint

$\overline{k}_n = 0$ imposed by $\delta(\overline{k}_n)$. By renaming the k's in (5.308) as:

$$\{k_1, k_2, \ldots, k_{n_3}\} \to \{k_{n-n_3+1}, k_{n-n_3+2}, \ldots, k_n\},$$
$$\{k_{n_3+1}, k_{n_3+2}, \ldots, k_n\} \to \{k_1, k_2, \ldots, k_{n-n_3}\}, \tag{5.309}$$

we deduce from (5.302) that $\Xi_1 = -\Lambda_2(k_1, \ldots, k_n)$. This indicates that the sum $\Lambda_2 + \Lambda_3$, being a term in $\Upsilon_4(k_1, \ldots, k_n)$, will contribute to $\widetilde{G}_c^{(n,3)}(k_1, \ldots, k_n)$ in the integration of (5.243) only by $\Xi_2(k_1, \ldots, k_n)$, which is free of any principal value distribution.

Now, if we substitute (5.278),(5.287), (5.289) and (5.291) for Υ_1, Υ_2, Υ_3 and Υ_4 respectively in the sum (5.266) and then insert the resultant sum into (5.264), we obtain:

$$\begin{aligned}
\widetilde{G}_c^{(n,3)}(k_1, \ldots, k_n) = & \sum_{\substack{n_1,n_2,n_3=2 \\ n_1+n_2+n_3=n}}^{n-4} \sum_{\nu=1}^{n_1-1} \sum_{\nu'=n_1+1}^{n_1+n_2-1} \Bigg[\prod_{\substack{\ell=1 \\ \ell \notin \{n_1, n_1+n_2\}}}^{n-1} \sum_{\mathfrak{m}_\ell=1}^{\infty} \Bigg] \\
& \frac{\triangle^{(n_1)}(\mathfrak{m}_1, \ldots, \mathfrak{m}_{n_1-1})}{\prod_{j=1}^{\nu} \left(E_{\mathfrak{m}_j} + i\left(\overline{k}_{n-j} - \overline{k}_{n-n_1}\right)\right) \prod_{\ell=\nu}^{n_1-1} \left(E_{\mathfrak{m}_\ell} + i\,\overline{k}_{n-\ell}\right)} \\
& \times \frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1}, \ldots, \mathfrak{m}_{n_1+n_2-1})}{\prod_{j=n_1+1}^{\nu'} \left(E_{\mathfrak{m}_j} + i\left(\overline{k}_{n-j} - \overline{k}_{n_3}\right)\right) \prod_{\ell=\nu'}^{n_1+n_2-1} \left(E_{\mathfrak{m}_\ell} + i\,\overline{k}_{n-\ell}\right)} \\
& \times \frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1}, .., \mathfrak{m}_{n-1})}{\prod_{\ell=n_1+n_2+1}^{n-1} \left(E_{\mathfrak{m}_\ell} + i\,\overline{k}_{n-\ell}\right)} + \sum_{\substack{n_1,n_2,n_3=2 \\ n_1+n_2+n_3=n}}^{n-4} \sum_{\nu=1}^{n_1-1} \sum_{\gamma=\nu}^{n_1-1} \Bigg[\prod_{\substack{\ell=1 \\ \ell \notin \{n_1, n_1+n_2\}}}^{n-1} \sum_{\mathfrak{m}_\ell=1}^{\infty} \Bigg] \\
& \frac{\triangle^{(n_1)}(\mathfrak{m}_1, \ldots, \mathfrak{m}_{n_1-1})}{\prod_{j=1}^{\nu} \left(E_{\mathfrak{m}_j} + i\left(\overline{k}_{n-j} - \overline{k}_{n-n_1}\right)\right) \prod_{\ell=\nu}^{\gamma} \left(E_{\mathfrak{m}_\ell} + i\left(\overline{k}_{n-\ell} - \overline{k}_{n_3}\right)\right) \prod_{\ell'=\gamma}^{n_1-1} \left(E_{\mathfrak{m}_{\ell'}} + i\,\overline{k}_{n-\ell'}\right)} \\
& \times \frac{\triangle^{(n_2)}(\mathfrak{m}_{n_1+1}, \ldots, \mathfrak{m}_{n_1+n_2-1})}{\prod_{\ell=n_1+1}^{n_1+n_2-1} \left(E_{\mathfrak{m}_\ell} + i\left(\overline{k}_{n-\ell} - \overline{k}_{n_3}\right)\right)} \frac{\triangle^{(n_3)}(\mathfrak{m}_{n_1+n_2+1}, \ldots, \mathfrak{m}_{n-1})}{\prod_{\ell'=n_1+n_2+1}^{n-1} \left(E_{\mathfrak{m}_{\ell'}} + i\,\overline{k}_{n-\ell'}\right)}.
\end{aligned} \tag{5.310}$$

Note that in calculating (5.310), we have redefined the summation index ν' in (5.291) as $\nu' \to n_1 + \nu'$, transforming the sum over ν' as:

$$\sum_{\nu'=1}^{n_2-1} \longrightarrow \sum_{\nu'=n_1+1}^{n_1+n_2-1}. \tag{5.311}$$

To encode our results in a single generic expression, we shall use the following notation:

$$X^{(n_j,s)}(k_1,k_2,\ldots,k_{n-\overline{n}_{j-1}-1}) = \Big[\prod_{\ell=1}^{s}\sum_{\substack{\nu_\ell=\nu_{\ell-1}\\ \nu_0=\overline{n}_{j-1}+1}}^{\overline{n}_j-1}\Big]\Big[\prod_{\ell=\overline{n}_{j-1}+1}^{\overline{n}_j-1}\sum_{\mathsf{m}_\ell=1}^{\infty}\Big]$$
$$\frac{\triangle^{(n_j)}(\mathsf{m}_{\overline{n}_{j-1}+1},\ldots,\mathsf{m}_{\overline{n}_j-1})}{\prod_{r=1}^{s}\left(E_{\mathsf{m}_{\nu_r}}+i\left(\overline{k}_{n-\nu_r}-\overline{k}_{n-\overline{n}_{j+r-1}}\right)\right)\prod_{\ell=\overline{n}_{j-1}+1}^{\overline{n}_j-1}\left(E_{\mathsf{m}_\ell}+i\left(\overline{k}_{n-\ell}-\overline{k}_{n-\sigma_\ell}\right)\right)}, \tag{5.312}$$

where σ_ℓ is a positive integer depending on n_j and ν_r as:

$$\sigma_\ell = \sigma_\ell(n_j;\nu_1,\nu_2,\ldots,\nu_s) = \begin{cases} \overline{n}_j & \text{if } \overline{n}_{j-1}+1 \le \ell < \nu_1 \\ \overline{n}_{j+1} & \text{if } \nu_1 \le \ell < \nu_2 \\ \overline{n}_{j+2} & \text{if } \nu_2 \le \ell < \nu_3 \\ \vdots & \vdots \\ \overline{n}_{j+s-1} & \text{if } \nu_{s-1} \le \ell < \nu_s \\ n & \text{if } \nu_s \le \ell \le \overline{n}_j - 1\,. \end{cases} \tag{5.313}$$

Here, $X^{(n_j,0)}$ is defined as:

$$X^{(n_j,0)}\left(\{k_{n-\overline{n}_j+r}\}_{r=1}^{n_j-1}\right) = \prod_{\ell'=\overline{n}_{j-1}+1}^{\overline{n}_j-1}\sum_{\mathsf{m}_{\ell'}=1}^{\infty}\frac{\triangle^{(n_j)}(\mathsf{m}_{\overline{n}_{j-1}+1},\ldots,\mathsf{m}_{\overline{n}_j-1})}{\prod_{\ell=\overline{n}_{j-1}+1}^{\overline{n}_j-1}\left(E_{\mathsf{m}_\ell}+i\left(\overline{k}_{n-\ell}-\overline{k}_{n-\overline{n}_j}\right)\right)}. \tag{5.314}$$

In this notation, we can rewrite (5.244), (5.256) and (5.310) as:

$$\widetilde{G}_c^{(n,1)}(k_1,\ldots,k_n) = X^{(n_1=n,0)}(k_1,\ldots,k_{n-1})\,, \tag{5.315}$$

$$\widetilde{G}_c^{(n,2)}(k_1,\ldots,k_n) = -\sum_{\substack{n_1,n_2=2\\ n_1+n_2=n}}^{n-2} X^{(n_1,1)}(k_1,\ldots,k_{n-1})\,X^{(n_2,0)}(k_1,\ldots,k_{n_2-1})\,, \tag{5.316}$$

$$\begin{aligned}\widetilde{G}_c^{(n,3)}(k_1,\ldots,k_n) =& \\ \sum_{\substack{n_1,n_2,n_3=2\\ n_1+n_2+n_3=n}}^{n-4} \Big[& X^{(n_1,1)}(k_1,\ldots,k_{n-1})\,X^{(n_2,1)}(k_1,\ldots,k_{n-n_1-1})\,X^{(n_3,0)}(k_1,\ldots,k_{n_3-1}) \\ & + X^{(n_1,2)}(k_1,\ldots,k_{n-1})\,X^{(n_2,0)}(k_{n_3+1},\ldots,k_{n_3+n_2-1})\,X^{(n_3,0)}(k_1,\ldots,k_{n_3-1})\Big]\,.\end{aligned} \tag{5.317}$$

It is now easy to deduce that these results are generated from the compact expression:

$$\widetilde{G}_c^{(n,r)}(k_1,\ldots,k_n) = (-1)^{r-1}\sum_{\substack{n_1,\ldots,n_r=2\\ n_1+\ldots+n_r=n}}^{n-2(r-1)}\ \sum_{\substack{s_1\geq s_2\ldots s_r\geq 0\\ s_1+\ldots+s_r=r-1}} X^{(n_1,s_1)}X^{(n_2,s_2)}\ldots X^{(n_r,s_r)}\,. \tag{5.318}$$

By testing this prescription for a few values of n in the case of $r=4$, we find its predictions to be consistent with the corresponding calculated results. This leads us to conjecture that (5.318) holds for all values of n and r. Following the same argument as in ref. [64], we claim that the sums over the non-zero energy eigenvalues in (5.318), or equivalently in $X^{(n_j,s_j)}$, are all convergent since the vacuum functional itself is considered as finite. Due to the absence of the vacuum energy contribution from the denominators of $X^{(n_j,s_j)}$, we can now Taylor expand $\widetilde{G}_c^{(n,r)}(k_1,\ldots,k_n)$ in the neighbourhood of the origin $(k_1,\ldots,k_n)=(0,\ldots,0)$, giving:

$$\widetilde{G}_c^{(n)}(k_1,\ldots,k_n) = \sum_{r=1}^{[n]}\widetilde{G}_c^{(n,r)}(k_1,\ldots,k_n) = \sum_{j_1,\ldots,j_n=0}^{\infty} C'_{j_1,\ldots,j_n}\,k_1^{j_1}\ldots k_n^{j_n}\,, \tag{5.319}$$

with $C'_{j_1,\ldots,j_n}$ being constant coefficients. This leads to the local expansion in (5.191), which is valid for any field $\varphi(x)$ having a Fourier transform $\widetilde{\varphi}(k)$ with a compact support of a sufficiently small size interval.

Now, let us focus on the analyticity properties of $\overline{W}_0[\widetilde{\varphi}]$ under the scale transformation of the source field $\widetilde{\varphi}\to\widetilde{\varphi}_s(k)=\sqrt{s}\,\widetilde{\varphi}(\sqrt{s}\,k)$, which corresponds to $\varphi\to\varphi_s(x)=\varphi(x/\sqrt{s}\,)$.

By evaluating $\overline{\mathsf{W}}_0[\widetilde{\varphi}]$ for the scaled field $\widetilde{\varphi}_s(k) = \sqrt{s}\ \widetilde{\varphi}(\sqrt{s}\ k)$ in the functional expansion:

$$\overline{\mathsf{W}}_0[\widetilde{\varphi}_s] = 2\pi \sum_{n=1}^{\infty} \int_{\mathbb{R}} \Big[\prod_{i=1}^{n} \frac{dk_i}{2\pi}\ \widetilde{\varphi}_s(k_i) \Big]\ \widetilde{G}_c^{(n)}(k_1, \ldots, k_n)\, \delta(k_1 + \cdots + k_n)\,, \tag{5.320}$$

and then changing the variables as $k_i \to \sqrt{s}\ k_i$ so that:

$$\overline{\mathsf{W}}_0[\widetilde{\varphi}_s] = \overline{\mathsf{W}}_0[\widetilde{\varphi}; s] = 2\pi \sum_{n=1}^{\infty} \int_{\mathbb{R}} \Big[\prod_{i=1}^{n} \frac{dk_i}{2\pi}\ \widetilde{\varphi}(k_i) \Big]\ \widetilde{G}_c^{(n)}(k_1, \ldots, k_n; s)\, \delta\Big(\sum_{i=1}^{n} k_i \Big)\,, \tag{5.321}$$

with $\widetilde{G}_c^{(n)}(k_1, \ldots, k_n; s) = \sqrt{s} \sum_{r=1}^{[n]} \widetilde{G}_c^{(n,r)}\big(\frac{k_1}{\sqrt{s}}, \ldots, \frac{k_n}{\sqrt{s}} \big)$, we find that the analyticity of $\overline{\mathsf{W}}_0[\widetilde{\varphi}_s]$ in the complex s-plane is determined by $\widetilde{G}_c^{(n)}(k_1, \ldots, k_n; s)$. The n-point function $\widetilde{G}_c^{(n)}(k_1, \ldots, k_n; s)$ acquires a dependence on the scaling parameter s via the functions $X^{(n_j, r_j)}$ whose s-dependence, when its arguments are all scaled as $k_i \to k_i/\sqrt{s}$, is given by:

$$X^{(n_j,r_j)} = s^{(r_j+n_j-1)/2} \Big[\prod_{\ell=1}^{r_j} \sum_{\substack{\nu_\ell=\nu_{\ell-1} \\ \nu_0=\overline{n}_{j-1}+1}}^{\overline{n}_j-1} \Big] \Big[\prod_{\ell=\overline{n}_{j-1}+1}^{\overline{n}_j-1} \sum_{\mathsf{m}_\ell=1}^{\infty} \Big]$$
$$\frac{\triangle^{(n_j)}(\mathsf{m}_{\overline{n}_{j-1}+1}, \ldots, \mathsf{m}_{\overline{n}_j-1})}{\prod_{l=1}^{r_j} \Big(\sqrt{s}\, E_{\mathsf{m}_{\nu_l}} + i\, (\overline{k}_{n-\nu_l} - \overline{k}_{n-\overline{n}_{j+l-1}}) \Big) \prod_{\ell=\overline{n}_{j-1}+1}^{\overline{n}_j-1} \Big(\sqrt{s}\, E_{\mathsf{m}_\ell} + i\, (\overline{k}_{n-\ell} - \overline{k}_{n-\sigma_\ell}) \Big)}\,. \tag{5.322}$$

This shows clearly that $\widetilde{G}_c^{(n)}(k_1, \ldots, k_n; s)$, or equivalently $\mathsf{W}_0[\varphi_s] = \overline{\mathsf{W}}_0[\widetilde{\varphi}_s]$, extends to an analytic function of s on the whole of the complex s-plane with a branch cut restricted to the negative real axis. This also applies to the vacuum functional itself since it is the exponential of $\mathsf{W}_0[\varphi_s]$.

Although we have described this calculation in detail for the case of scalar field theory in 1+1 dimensions, the method can be generalised straightforwardly to higher dimensions.

Chapter 6

Conclusions and outlook

In this thesis, we have developed a new approach for investigating physical observables of the type $F(Q^2)$ in regions that are inaccessible to perturbative methods of quantum field theory. In this approach, we have exploited the causality condition to reformulate $F(Q^2)$ as a limit as $\lambda \to \infty$ of a contour integral depending on λ. In this way, we have shown that the perturbatively violated analyticity structure of physical observables can be reinstated in, at least, the right half of the complex Q^2-plane by taking $\lambda = \lambda_e$ instead of ∞, where λ_e is the only free parameter of the theory. Explicit guidelines for finding an appropriate value for λ_e has been given with illustrative examples. We have also shown how our construction can play the role of a bridge between regions of small and large momenta, emphasising the fact that from a *prior* knowledge of either the UV or IR behaviour we can extract information about the IR or UV properties respectively. In fact, as our formalism incorporates non-perturbative effects it extends the range of applicability of perturbation theory to cover the whole energy domain.

We have demonstrated the implementation of our method in tackling the ghost-pole problem in QCD, giving a simple and new one-loop expression for the strong coupling constant. Furthermore, We have extended our calculations to include the exact Lambert W solution $\alpha^{(2)}_{LW}(Q^2)$ of the two-loop RG equation which suffers from an unphysical cut in the complex Q^2-plane. For this calculation, we have provided a detailed study of the singularity structure of $\alpha^{(2)}_{LW}(Q^2)$ which is essential for performing the contour integral in our representation of the coupling constant. Eventually, we have managed to remove the unwanted cut from the physical domain of the coupling constant without altering the

correct UV properties such as asymptotic freedom. Unlike the one-loop case, we do not obtain a simple expression for the coupling constant at the two-loop level. However, we can still easily read off the non-perturbative contributions in our model.

As our approach incorporates an extra free parameter λ_e in addition to Λ, we have included a special method of determining λ_e from the UV behaviour of either the λ-dependent coupling constant $\bar{\alpha}^{(n)}(q,\lambda)$ or its reciprocal $\bar{\chi}^{(n)}(q,\lambda)$. This method involves the calculation of the maximum curvature of $\bar{\alpha}^{(n)}(q,\lambda)$, or $\bar{\chi}^{(n)}(q,\lambda)$ for ease of computation, in the UV region $q > 1$ as explained and carried out numerically in section (2.3) and section (4.5) for the one- and two-loop cases respectively. In this framework, we have found the effective parameter λ_e to be 0.04 and 0.07 for $\bar{\alpha}^{(1)}(q,\lambda_e)$ and $\bar{\alpha}^{(2)}(q,\lambda_e)$ respectively. Although our prescription of obtaining λ_e via the maximum curvature procedure can be replaced by just tuning λ_e to allow the coupling fit with the experimental data available, we find our estimates for λ_e appropriate enough for our model, leading to a good agreement with the result $\alpha_s(Q^2) = 0.38 \pm 0.03(exp) \pm 0.04(theory)$ extracted from the fits to charmonium spectrum and fine structure splittings [37] at a low energy scale $Q = 1.0 \pm 0.2$ GeV. A supplementary discussion of how to determine the QCD scale parameter Λ in our model has also been considered.

A distinctive feature of our approach is that the running coupling freezes to a finite value at the origin $Q^2 = 0$, being consistent with a popular phenomenological hypothesis [22, 24] namely the IR freezing phenomenon. This has also been supported by Gribov theory of confinement which demonstrates how colour confinement can be achieved in a field theory of light fermions interacting with comparatively small effective coupling, a fact of potentially great impact for enlarging the domain of validity of perturbative ideology to the physics of hadrons and their interactions.

For illustration, we have carried out a comprehensive comparison between the predictions in our approach and those estimated by other theoretical methods. Besides, we have tested our model on a fit-invariant IR characteristic integral extracted from jet physics data [20, 38] over the energy interval $Q \leq 2\,\text{GeV}$. In section (3.2), this test shows a reasonable agreement with our prediction. For further applications, we have used our model for the running coupling to compute the gluon condensate and have shown that our result agrees very well with the value phenomenologically estimated from QCD sum rules [43]. Furthermore, we have calculated the $\beta-$function corresponding to our QCD coupling con-

stant and have shown that it behaves qualitatively like its perturbative counterpart, when calculated beyond the leading order and with a number of quark flavours allowing for the occurrence of IR fixed points. In further studies, it would be interesting to apply our analytic approach to improve the standard expressions for the running masses in perturbative QCD.

In chapter 5, we have illustrated a further application of our approach in Quantum field theory. We have given a simple example of reconstructing the free Schrödinger vacuum functional from a local expansion of its logarithm, being valid only for source fields $\varphi(x)$ whose Fourier transforms $\widetilde{\varphi}(k)$ are characterised by the support $\{k : |k| < m\}$, where m is the lightest mass in the theory. In this illustrative example, we have shown that the logarithm of the vacuum functional $\mathsf{W}_0[\varphi]$ under a scale transformation of the source field $\varphi(x) \to \varphi_s = \varphi(x/\sqrt{s})$ extends to an analytic function of s on the whole of the complex s-plane with a branch cut restricted to the negative real axis. This property of analyticity in the complex s-plane is the basis of our method because it allows the use of Cauchy's theorem for relating the large-s behaviour, where the local expansion of $\mathsf{W}_0[\varphi_s]$ holds, to the point $s = 1$.

Just as in the case of a free (massive) scalar field theory, we have shown that for an interacting scalar field theory with a non-zero mass gap the logarithm of the vacuum functional $\mathsf{W}_0[\varphi]$ reduces to a local expansion of the type (5.191) when the Fourier transform $\widetilde{\varphi}(k)$ of $\varphi(x)$ has a compact support of a sufficiently small size interval. A knowledge of this expansion or its leading terms enables us to estimate the vacuum $\Psi_0[\varphi] = \exp\big(\mathsf{W}_0[\varphi]\big)$ for an arbitrary source field by exploiting the analyticity of $\mathsf{W}_0[\varphi_s]$ in a complex scale parameter s. Our main concern, however, was not to compute the coefficients of this local expansion of $\mathsf{W}_0[\varphi]$ but to prove its existence and to show that the analytic structure of the scaled vacuum functional $\Psi_0[\varphi_s]$ in the complex s-plane is the same as its counterpart in the free field theory.

To justify the existence of a local expansion for $\mathsf{W}_0[\varphi]$, we had to show that all the energy denominators associated with the zero-point energy in the disconnected n-point functions $\widetilde{\mathfrak{J}}_d^{(n)}(k_1, \ldots, k_n)$ cancel when combined in a finite sum to form the connected n-point functions $\widetilde{G}_c^{(n)}(k_1, \ldots, k_n)$, which determines the nth term $\mathsf{W}_0^{(n)}[\varphi]$ in the Taylor functional expansion of $\mathsf{W}_0[\varphi]$. In this way, the singular behaviour as $(k_1, \ldots, k_n) \to (0, \ldots, 0)$ disappears and a Taylor series for $\widetilde{G}_c^{(n)}(k_1, \ldots, k_n)$ around the origin is obtainable with a

non-zero radius of convergence. This grants $\mathsf{W}_0[\varphi]$ a local functional expansion, valid for fields $\varphi(x)$ whose Fourier transforms $\widetilde{\varphi}(k)$ have a sufficiently small support. In addition to this, the regularity of $\widetilde{G}_c^{(n)}(k_1,\ldots,k_n)$ at the origin is essential to study its analyticity in the complex s-plane for the scaled momenta $k_j \to k_j/\sqrt{s}$. We have shown that $\widetilde{G}_c^{(n)}(k_1/\sqrt{s},\ldots,k_n/\sqrt{s})$ acquires a dependence on s via non-singular energy denominators of general form $1/\big(E_\ell + i(\sum k_j)/\sqrt{s}\,\big)$, where E_ℓ is a non-zero energy eigenvalue. From this, we have deduced that the scaled functional $\mathsf{W}_0^{(n)}[\varphi_s] = \mathsf{W}_0^{(n)}[\varphi;s]$, associated with $\widetilde{G}_c^{(n)}$, continues to an analytic function of s on the whole of the complex s-plane with the negative real axis removed. By exploiting this property of analyticity in the complex scaling parameter s, we have shown how the vacuum functional for an arbitrary source $\varphi(x)$ can be reconstructed from a given local expansion of its logarithm, which is valid only for source fields whose Fourier transforms have small supports.

We have described this calculation in detail for the case of scalar field theory in 1+1 dimensions, although the method generalises to higher dimensions, and to other field theories by modifying the coupling term in (5.207). For example, the Yang-Mills vacuum functional (in the Weyl-gauge $A_0 = 0$) is obtained by replacing $\varphi(x)\,\dot{\phi}(x,0)$ and $S_E[\phi]$ in (5.207) by $(\mathbf{A}-\mathcal{A}).\dot{\mathcal{A}}$ and the Yang-Mills action $S_{YM}[\mathcal{A}]$, respectively, and then integrating over the gauge field $\mathcal{A}$ to leave a functional of $\mathbf{A}$, $\Psi_0[\mathbf{A}]$, see ref. [65]. In this way, we could in principal extend our method to discuss the analyticity of the Yang-Mills vacuum functional and its local expansion. This approach provides a new analytical framework to study physics beyond perturbation theory.

Appendix A

contour integrations around the branch points of $\mathcal{W}$ and the simple pole at $k = q$

In this appendix, we shall be involved with contour integrals of the type:

$$I_{\widetilde{\gamma}} = \frac{1}{2\pi i} \int_{\widetilde{\gamma}} \frac{\mathrm{e}^{\lambda(k-q)}}{(k-q)} \, \mathcal{W}(k) \, dk \,, \tag{A.1}$$

where $\widetilde{\gamma}$ is an arbitrary smooth curve in the complex $k-$plane, not crossing the branch cuts of $\mathcal{W}(k)$. Our main task here is to show that in the limit $\epsilon \to 0$ we obtain the following results:

1. for $\widetilde{\gamma} = \gamma_1^{\pm}$, $I_{\widetilde{\gamma}} \to 0$ if $q \neq 0$;

2. for $\widetilde{\gamma} = \gamma$, $I_{\widetilde{\gamma}} \to 0$ if $q \neq 1$ otherwise $I_{\widetilde{\gamma}} \to \mathcal{W}(1) = -1$;

3. for $\widetilde{\gamma} = \gamma_2^{\pm}$, $I_{\gamma_2^+} \to \frac{1}{2}\mathcal{W}(q)$ and $I_{\gamma_2^-} \to \frac{1}{2}\mathcal{W}^*(q)$ if $q \neq 0$;

where the relevant contours $\gamma_1^{\pm}$, $\gamma_2^{\pm}$ and γ together with the radius ϵ are as depicted in Fig.(4.3) and Fig.(4.4).

We begin by considering the case in which the contour $\widetilde{\gamma}$ in (A.1) is given by the semicircular arc γ_1^+. In this case, the path of integration is parametrised by:

$$k = \epsilon \, \mathrm{e}^{i\theta} \,, \qquad 0 \leq \theta \leq \pi \,. \tag{A.2}$$

Hence, by use of (A.2), we have:

$$I_{\gamma_1^+} = \frac{\epsilon\, e^{-\lambda q}}{2\pi} \int_0^{\pi} \frac{e^{\lambda\epsilon\cos\theta}\, e^{i\lambda\epsilon\sin\theta}}{\epsilon - q\, e^{-i\theta}}\, W_{-1}(e^{-1-\upsilon\ln\epsilon}\, e^{i(\pi-\upsilon\theta)})\, d\theta\,. \tag{A.3}$$

Now, from the following inequalities:

$$\frac{1}{|\epsilon - q\, e^{-i\theta}|} \leq \frac{1}{|q-\epsilon|}\,, \qquad e^{\lambda\epsilon\cos\theta} \leq e^{\lambda\epsilon}\,, \tag{A.4}$$

$$\left| W_{-1}(e^{-1-\upsilon\ln\epsilon}\, e^{i(\pi-\upsilon\theta)}) \right| \leq \left| W_{-1}(e^{-1-\upsilon\ln\epsilon}\, e^{i\pi(1-\upsilon)}) \right|, \quad (0 \leq \theta \leq \pi)\,, \tag{A.5}$$

we deduce that:

$$|I_{\gamma_1^+}| \leq \frac{e^{-\lambda(q-\epsilon)}}{2|q-\epsilon|}\, \mathcal{M}(\epsilon)\,, \tag{A.6}$$

where

$$\mathcal{M}(\epsilon) = \epsilon \left| W_{-1}(e^{-1-\upsilon\ln\epsilon}\, e^{i\pi(1-\upsilon)}) \right|. \tag{A.7}$$

Since $W_n(z)$ tends to the nth branch of the complex logarithm $L_n(z) = \ln(z) + i\,2\pi\,n$ at very large $|z|$, we find that:

$$W_{-1}(e^{-1-\upsilon\ln\epsilon}\, e^{i(\pi-\upsilon\theta)}) \cong -1 - \upsilon\ln\epsilon - i\,(\pi + \upsilon\theta)\,, \tag{A.8}$$

for infinitesimally small ϵ. This, together with (4.19), allows us to evaluate the limit of (A.7) as $\epsilon \to 0$, giving:

$$\lim_{\epsilon\to 0} \mathcal{M}(\epsilon) = 0\,. \tag{A.9}$$

As a result of this, it follows from (A.6) that in the limit $\epsilon \to 0$ the integral $I_{\gamma_1^+}$ tends to zero provided that $q \neq 0$. Now, we shall show that the argument used above on $I_{\gamma_1^+}$ applies equally well to $I_{\gamma_1^-}$, yielding the same result. In this case, using (A.2) to parametrise γ_1^- in the lower half-plane $-\pi < \theta < 0$, we obtain:

$$I_{\gamma_1^-} = \frac{\epsilon\, e^{-\lambda q}}{2\pi} \int_{-\pi}^{0} \frac{e^{\lambda\epsilon\cos\theta}\, e^{i\lambda\epsilon\sin\theta}}{\epsilon - q\, e^{-i\theta}}\, W_1(e^{-1-\upsilon\ln\epsilon}\, e^{-i(\pi+\upsilon\theta)})\, d\theta\,. \tag{A.10}$$

By use of (A.4) and the fact that:

$$\left| W_1(e^{-1-\upsilon\ln\epsilon}\, e^{-i(\pi+\upsilon\theta)}) \right| \leq \left| W_1(e^{-1-\upsilon\ln\epsilon}\, e^{-i\pi(1-\upsilon)}) \right|, \quad (-\pi \leq \theta \leq 0)\,, \tag{A.11}$$

we arrive at:

$$|I_{\gamma_1^-}| \leq \frac{\mathrm{e}^{-\lambda(q-\epsilon)}}{2|q-\epsilon|}\,\mathcal{N}(\epsilon)\,, \tag{A.12}$$

where

$$\mathcal{N}(\epsilon) = \epsilon\left|W_1(\mathrm{e}^{-1-\upsilon\ln\epsilon}\,\mathrm{e}^{-i\pi(1-\upsilon)})\right|. \tag{A.13}$$

Since $W_1(\mathrm{e}^{-1-\upsilon\ln\epsilon}\,\mathrm{e}^{-i\pi(1-\upsilon)})$ behaves exactly like $(-1-\upsilon\ln\epsilon)+i\pi\,(1+\upsilon)$ for sufficiently small ϵ, it is not difficult to show that:

$$\lim_{\epsilon\to 0}\mathcal{N}(\epsilon) = 0\,. \tag{A.14}$$

Hence, by taking the limit $\epsilon \to 0$ in (A.12) we conclude that:

$$\lim_{\epsilon\to 0} I_{\gamma_1^-} = 0 \qquad \text{for } q \neq 0\,. \tag{A.15}$$

Now, we shall consider the contour integral (A.1) along the circular path $\widetilde{\gamma} = \gamma$, showing that for $q \neq 1$ the integral $I_\gamma \to 0$ as $\epsilon \to 0$. The parametrisation of γ by $k = 1 + \epsilon\,\mathrm{e}^{i\phi}$, where $-\pi < \phi \leq \pi$, allows us to write:

$$I_\gamma = \frac{\epsilon\,\mathrm{e}^{\lambda(1-q)}}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{e}^{\lambda\epsilon\cos\phi}\,\mathrm{e}^{i\lambda\epsilon\sin\phi}}{\epsilon+(1-q)\mathrm{e}^{-i\phi}}\,\mathcal{W}(1+\epsilon\,\mathrm{e}^{i\phi})\,d\phi\,. \tag{A.16}$$

From (A.4) and the fact that:

$$\left|\mathcal{W}(1+\epsilon\,\mathrm{e}^{i\phi})\right| \leq \left|\mathcal{W}(1+\epsilon)\right| = -W_{-1}(\mathrm{e}^{-1-\upsilon\ln\sqrt{1+2\epsilon+\epsilon^2}}\,\mathrm{e}^{i\pi}) \geq 1\,, \tag{A.17}$$

we can show that:

$$|I_\gamma| \leq -\frac{\epsilon\,\mathrm{e}^{-\lambda(q-1-\epsilon)}}{|\,|q-1|-\epsilon\,|}\,W_{-1}(\mathrm{e}^{-1-\upsilon\ln\sqrt{1+2\epsilon+\epsilon^2}}\,\mathrm{e}^{i\pi})\,. \tag{A.18}$$

By taking the limit $\epsilon \to 0$ in (A.18), recalling that $W_{-1}(\mathrm{e}^{-1}\,\mathrm{e}^{i\pi}) = -1$, we deduce that:

$$\lim_{\epsilon\to 0} I_\gamma = 0 \qquad \text{for } q \neq 1\,. \tag{A.19}$$

Also, we observe from (A.18) that if $q = 1$ then $|I_\gamma| \leq 1$ in the limit $\epsilon \to 0$. For the case $q = 1$, (A.16) reduces to:

$$I_\gamma = \frac{1}{2\pi} \int_{-\pi}^{\pi} f_n(\phi)\, d\phi\,, \tag{A.20}$$

where $n = 1/\epsilon$ and:

$$f_n(\phi) = \mathrm{e}^{\lambda n^{-1} \cos\phi} \mathrm{e}^{i\lambda n^{-1} \sin\phi}\ \mathcal{W}(1 + n^{-1}\, \mathrm{e}^{i\,\phi})\,. \tag{A.21}$$

Since $f_n(\phi)$ converges uniformly[1] to $\mathcal{W}(1) = -1$ on the real interval $-\pi < \phi \leq \pi$, we can pass the limit $n \to \infty$ through the integration sign in (A.20), obtaining:

$$\lim_{\epsilon \to 0} I_\gamma = \lim_{n \to \infty} I_\gamma = \frac{1}{2\pi} \int_{-\pi}^{\pi} \lim_{n \to \infty} f_n(\phi)\, d\phi\ = \mathcal{W}(1) = -1\,. \tag{A.22}$$

Let us now consider the contour integral (A.1) along the semicircular arc γ_2^+, proving that $I_{\gamma_2^+} \to \frac{1}{2}\mathcal{W}(q)$ as $\epsilon \to 0$ for any $q > 0$. To achieve this result, we begin by parametrising the contour of integration γ_2^+ according to $k = q + \epsilon\, \mathrm{e}^{i\,\varphi}$, giving:

$$I_{\gamma_2^+} = \frac{1}{2\pi} \int_0^{\pi} \mathrm{e}^{\lambda\epsilon \cos\varphi} \mathrm{e}^{i\lambda\epsilon \sin\varphi}\ \mathcal{W}(q + \epsilon\, \mathrm{e}^{i\,\varphi})\, d\varphi\,. \tag{A.23}$$

Here, given $\varphi \in [0, \pi]$, we write:

$$\mathcal{W}(q + \epsilon\, \mathrm{e}^{i\,\varphi}) = W_{-1}(\mathrm{e}^{-1 - \upsilon \ln\mathcal{R}(\epsilon,\varphi)}\ \mathrm{e}^{i(\pi - \upsilon\Theta(\epsilon,\varphi))})\,, \tag{A.24}$$

where

$$\mathcal{R}(\epsilon, \varphi) = \sqrt{q^2 + 2q\epsilon\cos\varphi + \epsilon^2}\,, \qquad \Theta(\epsilon, \varphi) = \arctan\left(\frac{\epsilon \sin\varphi}{q + \epsilon\cos\varphi}\right). \tag{A.25}$$

Since the integrand in (A.23) is a continuous complex-valued function on the real interval $0 \leq \varphi \leq \pi$, we use the mean value theorem to obtain:

$$I_{\gamma_2^+} = \frac{1}{2}\, \mathrm{e}^{\lambda\epsilon\cos\widehat{\varphi}}\, \mathrm{e}^{i\lambda\epsilon\sin\widehat{\varphi}}\, W_{-1}(\mathrm{e}^{-1 - \upsilon \ln\mathcal{R}(\epsilon,\widehat{\varphi})}\ \mathrm{e}^{i(\pi - \upsilon\Theta(\epsilon,\widehat{\varphi}))})\,, \tag{A.26}$$

[1] By $f_n(\phi)$ being uniformly convergent to $\mathcal{W}(1)$ on $(-\pi, \pi]$, we mean that $\sup\{|f_n(\phi) - \mathcal{W}(1)| : -\pi < \phi \leq \pi\} = |\mathrm{e}^{\lambda/n}\ \mathcal{W}(1 + 1/n) - \mathcal{W}(1)| \to 0$ as $n \to \infty$ (i.e. $\epsilon \to 0$), where $\sup \mathcal{S}$ denotes the supremum or the least upper bound of the given set $\mathcal{S}$.

where $0 \leq \widehat{\varphi}(\epsilon, \lambda) \leq \pi$. If we now take the limit $\epsilon \to 0$, we arrive at the required result:

$$\lim_{\epsilon \to 0} I_{\gamma_2^+} = \frac{1}{2}\, W_{-1}(\mathrm{e}^{-1-v \ln q}\, \mathrm{e}^{i\pi}) = \frac{1}{2}\, \mathcal{W}(q)\,, \qquad q \neq 0\,. \tag{A.27}$$

This could have been obtained also by passing the limit $\epsilon \to 0$ through the integration sign in (A.23), just as we did earlier in (A.22), since the integrand there converges uniformly to $\mathcal{W}(q)$.

Now, following the same argument used in deriving (A.27) we can immediately show that when $\widetilde{\gamma} = \gamma_2^-$ in (A.1) we have:

$$\begin{aligned} \lim_{\epsilon \to 0} I_{\gamma_2^-} &= \frac{1}{2\pi} \lim_{\epsilon \to 0} \int_{-\pi}^{0} \mathrm{e}^{\lambda \epsilon \cos\varphi} \mathrm{e}^{i\lambda\epsilon \sin\varphi}\; \mathcal{W}(q + \epsilon\, \mathrm{e}^{i\,\varphi})\; d\varphi \\ &= \frac{1}{2}\, W_{-1}^{*}(\mathrm{e}^{-1-v \ln q}\, \mathrm{e}^{i\pi}) = \frac{1}{2}\, \mathcal{W}^{*}(q)\,, \qquad q \neq 0\,. \end{aligned} \tag{A.28}$$

From (A.27) and (A.28) it follows that:

$$\lim_{\epsilon \to 0} \left(I_{\gamma_2^+} + I_{\gamma_2^-} \right) = \mathrm{Re}\,\{\mathcal{W}(q)\} \qquad \text{for } \; q > 0\,. \tag{A.29}$$

Appendix B

Green's Function with Dirichlet Boundary Conditions

Green's functions provide a useful method for solving inhomogeneous differential equations subject to some boundary conditions. We shall apply this method to the partial differential equation (5.138), which we relabel as:

$$(-\partial^2 + m^2)\phi_c(x) = \sigma(x), \qquad \sigma(x) = \rho(x) + 2\,\dot{\delta}(t)\,\varphi(\mathbf{x}), \qquad \partial^2 = \frac{\partial^2}{\partial t^2} + \nabla^2, \tag{B.1}$$

subject to the Dirichlet boundary conditions:

$$\phi_c(x)\big|_{t=0} = \phi_c(\mathbf{x}, 0) = 0\,, \qquad \phi_c(x)\big|_{t=-\infty} = \phi_c(\mathbf{x}, -\infty) = 0\,. \tag{B.2}$$

The first derivative of the Dirac δ-function $\dot{\delta}(t)$ can be defined as the limit of $\alpha(t,\epsilon)$ as $\epsilon \to 0$, where

$$\alpha(t,\epsilon) = \begin{cases} -\dfrac{1}{2\epsilon}\,\mathrm{P}\Big(\dfrac{1}{t}\Big) & \text{if } |t| \le \epsilon\,, \\ 0 & \text{if } |t| > \epsilon\,, \end{cases} \qquad \mathrm{P}\Big(\frac{1}{t}\Big) = \begin{cases} \dfrac{1}{t} & \text{if } t \neq 0\,, \\ 0 & \text{if } t = 0\,. \end{cases} \tag{B.3}$$

Note that for $t \in (-\infty, -\epsilon)$, with ϵ being infinitesimally small, it follows from (B.1) that $\sigma(\mathbf{x}, t) = \rho(\mathbf{x}, t)$ which we assume to be continuous on this time interval. However, for $t = 0$ we can always choose $\rho(\mathbf{x}, t)$ such that $\sigma(\mathbf{x}, t)$ is finite.

The formal solution of (B.1) can be expressed in terms of the Green's function $G_D(\mathbf{x}, t\,; \mathbf{x}', t')$

as:

$$\phi_c(\mathbf{x},t) = \int_\Gamma d^4x' \;\; G_D(\mathbf{x},t\,;\mathbf{x}',t')\;\sigma(\mathbf{x}',t')\,, \tag{B.4}$$

where $G_D(\mathbf{x},t\,;\mathbf{x}',t')$ satisfies:

$$\Big(-\frac{\partial^2}{\partial t^2} - \nabla^2 + m^2\Big)\, G_D(\mathbf{x},t\,;\mathbf{x}',t') = \delta(\mathbf{x}-\mathbf{x}')\,\delta(t-t')\,, \tag{B.5}$$

and the Dirichlet boundary conditions:

$$G_D(\mathbf{x},0\,;\mathbf{x}',t') = 0\,, \qquad G_D(\mathbf{x},-\infty\,;\mathbf{x}',t') = 0\,. \tag{B.6}$$

With no restriction on $G_D(\mathbf{x},t\,;\mathbf{x}',t')$ from its spatial coordinates, which are defined on the whole of $\mathbb{R}^3$, and with a δ-function source $\delta(\mathbf{x}-\mathbf{x}')$ appearing in (B.5), which depends only on the coordinate differences, it is clear that:

$$G_D(\mathbf{x},t\,;\mathbf{x}',t') = G_D(\mathbf{x}-\mathbf{x}';t,t')\,. \tag{B.7}$$

By making use of the integral Fourier transforms:

$$G_D(\mathbf{x}-\mathbf{x}';t,t') = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\;\widetilde{G}_D(\mathbf{k}\,;t,t')\;\mathrm{e}^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}')}\,, \tag{B.8}$$

$$\delta(\mathbf{x}-\mathbf{x}') = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\;\mathrm{e}^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}')}\,, \tag{B.9}$$

we can reduce (B.5) to a one-dimensional differential equation in time:

$$\Big(-\frac{\partial^2}{\partial t^2} + \omega^2\Big)\widetilde{G}_D(\mathbf{k}\,;t,t') = \delta(t-t'), \qquad \omega = \sqrt{\mathbf{k}^2+m^2}, \tag{B.10}$$

subject to the Dirichlet boundary conditions:

$$\widetilde{G}_D(\mathbf{k}\,;0,t') = 0\,, \qquad \widetilde{G}_D(\mathbf{k}\,;-\infty,t') = 0\,. \tag{B.11}$$

For $t \neq t'$, the differential equation in (B.10) becomes homogeneous and reduces to:

$$\Big(-\frac{\partial^2}{\partial t^2} + \omega^2\Big)\widetilde{G}_D(\mathbf{k}\,;t,t') = 0\,, \tag{B.12}$$

which has the solution:

$$\widetilde{G}_D(\mathbf{k}\,;t,t') = \begin{cases} \mathcal{G}_1(\mathbf{k};t,t') = a_1(\mathbf{k},t')\,\mathrm{e}^{\omega t} + a_2(\mathbf{k},t')\,\mathrm{e}^{-\omega t} & \text{for } t > t'\,, \\ \mathcal{G}_2(\mathbf{k};t,t') = b_1(\mathbf{k},t')\,\mathrm{e}^{\omega t} + b_2(\mathbf{k},t')\,\mathrm{e}^{-\omega t} & \text{for } t < t'\,. \end{cases} \tag{B.13}$$

Applying the Dirichlet boundary conditions (B.11) to this solution gives:

$$\widetilde{G}_D(\mathbf{k};t,t') = \begin{cases} \mathcal{G}_1(\mathbf{k};t,t') = a(\mathbf{k},t')\left[\mathrm{e}^{\omega t} - \mathrm{e}^{-\omega t}\right] & \text{for } t > t'\,, \\ \mathcal{G}_2(\mathbf{k};t,t') = b(\mathbf{k},t')\,\mathrm{e}^{\omega t} & \text{for } t < t'\,. \end{cases} \tag{B.14}$$

Integrating both sides of the differential equation in (B.10) over an infinitesimal interval $t \in [t'-\epsilon, t'+\epsilon]$, and assuming that $\widetilde{G}_D(\mathbf{k};t,t')$ is bounded there leads to:

$$\frac{d}{dt}\,\mathcal{G}_1(\mathbf{k};t,t')\Big|_{t=t'} - \frac{d}{dt}\,\mathcal{G}_2(\mathbf{k};t,t')\Big|_{t=t'} = -1\,, \tag{B.15}$$

which together with the continuity condition imposed on $\widetilde{G}_D(\mathbf{k};t,t')$ at $t=t'$, namely:

$$\mathcal{G}_1(\mathbf{k};t,t')\Big|_{t=t'} = \mathcal{G}_2(\mathbf{k};t,t')\Big|_{t=t'}\,, \tag{B.16}$$

determines the coefficients $a(\mathbf{k},t')$ and $b(\mathbf{k},t')$ in (B.14), giving:

$$a(\mathbf{k},t') = -\frac{1}{2\,\omega}\;\mathrm{e}^{\omega t'}\,, \qquad b(\mathbf{k},t') = -\frac{1}{2\,\omega}\left(\mathrm{e}^{\omega t'} - \mathrm{e}^{-\omega t'}\right). \tag{B.17}$$

By substituting this in (B.14), we obtain:

$$\widetilde{G}_D(\mathbf{k};t,t') = \begin{cases} \mathcal{G}_1(\mathbf{k};t,t') = -\frac{1}{2\omega}\left[\mathrm{e}^{\omega(t+t')} - \mathrm{e}^{-\omega(t-t')}\right] & \text{for } t > t'\,, \\ \mathcal{G}_2(\mathbf{k};t,t') = -\frac{1}{2\omega}\left[\mathrm{e}^{\omega(t+t')} - \mathrm{e}^{-\omega(t'-t)}\right] & \text{for } t < t'\,. \end{cases} \tag{B.18}$$

By making use of the Heaviside step function:

$$\theta(t) = \begin{cases} 1 & \text{for } t > 0\,, \\ 0 & \text{for } t < 0\,, \\ \frac{1}{2} & \text{for } t = 0\,, \end{cases} \qquad \theta(t) + \theta(-t) = 1\,, \tag{B.19}$$

we can rewrite (B.18) as:

$$\widetilde{G}_D(\mathbf{k};t,t') = \mathcal{G}_1(\mathbf{k};t,t')\,\theta(t-t') + \mathcal{G}_2(\mathbf{k};t,t')\,\theta(t'-t)\,, \tag{B.20}$$

which we can simplify to:

$$\widetilde{G}_D(\mathbf{k};t,t') = -\frac{1}{2\,\omega}\left[\,\mathrm{e}^{\omega(t+t')} - \mathrm{e}^{-\omega|t-t'|}\,\right]. \tag{B.21}$$

It is straightforward to chick that (B.21) satisfies the Dirichlet boundary conditions given in (B.11). With the help of the integral Fourier transform:

$$\frac{\mathrm{e}^{-\omega|\tau|}}{2\,\omega} = \int_{-\infty}^{\infty}\frac{dk_0}{2\pi}\;\frac{1}{k_0^2+\omega^2}\;\mathrm{e}^{ik_0\tau}\,, \tag{B.22}$$

we can find an integral representation for (B.21):

$$\widetilde{G}_D(\mathbf{k};t,t') = \int_{-\infty}^{\infty}\frac{dk_0}{2\pi}\;\frac{\mathrm{e}^{ik_0(t-t')} - \mathrm{e}^{ik_0(t+t')}}{k_0^2+\omega^2}\,. \tag{B.23}$$

Substituting this in (B.8) gives:

$$G_D(\mathbf{x}-\mathbf{x}';t,t') = \Delta_F(\mathbf{x}-\mathbf{x}';t-t') - \Delta_F(\mathbf{x}-\mathbf{x}';t+t')\,, \tag{B.24}$$

where $\Delta_F(\mathbf{y};y_0)$ is the well-known Feynman propagator in Euclidean space-time:

$$\Delta_F(\mathbf{y};y_0) = \int_{\mathbb{R}^4}\frac{d^4k}{(2\pi)^4}\;\frac{1}{k^2+m^2}\;\mathrm{e}^{ik_0y_0+i\mathbf{k}.\mathbf{y}}\,,\qquad k^2 = k_0^2+\mathbf{k}^2\,. \tag{B.25}$$

This shows that:

$$G_D(\mathbf{x},t;\mathbf{x}',t') = G_D(\mathbf{x}',t';\mathbf{x},t)\,. \tag{B.26}$$

Bibliography

[1] T. Muta, Foundations of Quantum Chromodynamics, World Scientific, 1987.

[2] M. Chaichian and N. F. Nelipa, Introduction to Gauge Field Theories, Springer-Verlag, 1984.

[3] Michael E. Peskin and Daniel V. Schroeder, An Introduction to Quantum Field Theory, Addison-Wesley, 1995

[4] J. D. Jackson, Classical Electrodynamics, Jonn Wiley & Sons, Second Edition 1975.

[5] R. A. Bertlmann, Anomalies in Quantum Field Theory, Clarendon Press, 1996.

[6] I. Jack and H. Osborn, Nucl. Phys. B207 (1982) 474.

[7] H. Osborn, Lectures on Gauge Theory Methods in " The Standard Model and Beyond ", ed., W. J. Zakrzewski, Adam Hilger, 1987.

[8] L. F. Abbott, Acta Phys. Polon. B13 (1982) 33; Nucl. Phys. B185 (1981) 189.

[9] S. Pokorski, Gauge Field Theories, Cambridge university press, Second edition, 2000.

[10] E. Corrigan, P. Goddard, H. Osborn and S. Templeton, Nucl. Phys. B159 (1979) 469; E. Corrigan and P. Goddard, Some Aspects of Instantons, Lectures given at Canadian Mathematical Society Meeting, Montreal, Canada,Sep. 3-8, 1979, Published in Lecture Notes in Physics (129).

[11] I. L. Buchbinder, S. D. Odintsov and I. L. Shapiro, Effective Action in Quantum Gravity, Institute of Physics (IOP) Publishing Ltd, 1992.

[12] H.D.Politzer, Phys. Rev. Lett. 30 (1973) 1346; D. J. Gross and F. Wilczek, Phys. Rev. Lett. 30 (1973) 1343.

[13] G. Paris, Phys. Lett. B76 (1978) 65; Phys. Lett. B 69 (1977) 109.

[14] Yu. A. Simonov, Phys. Atom. Nucl. 58 (1995) 107; Yu. A. Simonov, JETP Lett. 57 (1993) 525.

[15] A. M. Badalian and Yu. A. Simonov, Phys. Atom. Nucl. 60 (1997) 630.

[16] G. Grunberg, Phys. Lett. B372 (1996) 121.

[17] E. Gardi, M. Karliner and G. Grunberg, JHEP07 (1998) 007; hep-ph/9806462.

[18] B. R. Webber, JHEP 9810 (1998) 012 (hep-th/9805484).

[19] D. V. Shirkov and I. L. Solovtsov, Phys. Rev. Lett. 79 (1997) 1209 (hep-ph/9704333); I. L. Solovtsov and D. V. Shirkov, hep-ph/9909305.

[20] Yu. L. Dokshitzer, V. A. Khoze and S. I. Troyan, Phys. Rev. D53 (1996) 89 (hep-ph/9506425).

[21] A. I. Alekseev and B. A. Arbuzov, hep-ph/9704228

[22] A. C. Mattingly and P. M. Stevenson, Phys. Rev. D 49 (1994) 437; Phys. Rev. Lett. 69 (1992) 1320

[23] J. Nyiri, The Gribov Theory of Quark Confinement, World Scientific 2001.

[24] P. M. Stevenson, Phys. Lett. B331 (1994) 187.

[25] F. Close et al., Phys. Lett. B319 (1993) 291; V. N. Gribov, Lund preprint LU-TP 91-7 (March 1991).

[26] M. Shifman, ed., At the frontier of particle physics-Handbook of QCD, Vol. 1, World Scientific, 2001.

[27] H. W. Wyld, Mathematical Methods for Physics, Perseus Books 1999.

[28] G. Arfken, Mathematical Methods for Physicists, Academic Press 1985; A. Erdélyi et al., Higher Transcendental Functions, Vol. 2, McGraw-Hill Book Company, 1953.

[29] F. I. Ynduráin, The Theory of Quark and Gluon Interactions, Springer 1999.

[30] S. A. Larin and J. A. M. Vermaseren, Phys. Lett. B303 (1993) 334.

[31] J. G. Körner, F. Krajewski and A. A. Pivovarov, Phys. Rev. D63 (2001) 036001; hep-ph/0002166

[32] E. Tournefier, Proc. of the Quarks '98 Int. Seminar, Suzdal, Russia, May 1998; hep-ex/9810042

[33] The LEP Collaborations ALEPH, DELPHI, L3, OPAL, the LEP Electroweak Working Group and the SLD Heavy Flavour and Electroweak Groups, CERN-EP/2000-016.

[34] K. G. Chetyrkin, J. H. Kühn and M. Steinhauser, hep-ph/0004189

[35] S. Capitani, M. Lüscher, R. Sommer and H. Wittig, Nucl. Phys. B544 (1999) 669.

[36] W. J. Marciano, Phys. Rev. D29 (1984) 580.

[37] A. M. Badalian and V. L. Morgunov, Phys. Rev. D60 (1999) 116008; hep-ph/9901430

[38] Yu. L. Dokshitzer and B. R. Webber, Phys. Lett. B352 (1995) 451.

[39] Yu. L. Dokshitzer, hep-ph/9812252; A. I. Alekseev, hep-ph/9802372.

[40] V. Gogohia and H. Toki, Phys. Lett. B466 (1999) 305.

[41] M. A. Shifman, Phys. Rep. 209 (1991) 341.

[42] C. Bernard, Phys. Rev. D19 (1979) 3013.

[43] M. A. Shifman, A. I. Vainshtein and V. I. Zakharov, Nucl. Phys. B147 (1979) 385; 448.

[44] B. Guberina, R. Meckbach, R. D. Peccei and R. Rückl, Nucl. Phys. B184 (1981) 476.

[45] R. K. Ellis, W. J. Stirling and B. R. Webber, QCD and Collider Physics, Cambridge University Press, 1996.

[46] T. van Ritbergen, J. A. M. Vermaseren and S. A. Larin, Phys. Lett. B400 (1997) 379; hep-ph/9701390.

[47] R. E. Marshak, Conceptual Foundations of Modern Particle Physics, World Scientific, 1993.

[48] R. M. Corless, G. H. Gonnet, D. E. G. Hare, D. J. Jeffrey and D. E. Knuth, Advances in Computational Mathematics 5 (1996) 329-359.

[49] R. L. Graham, D. E. Knuth and O. Patashnik, Concrete Mathematics, Addison-Wesley 1994.

[50] D. J. Jeffrey, R. M. Corless, D. E. G. Hare and D. E. Knuth, "Sur l'inversion de $y^{\alpha}\, e^{y}$ au moyen de nombres de Stirling associés" , C. R. Acad. Sc. Paris, Série I, 320 (1995) 1449-1452.

[51] I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series, and Products, Academic Press, 1980.

[52] B. Hatfield, Quantum field theory of point particles and strings, Addison-Wesley, 1992.

[53] R. Jackiw, Analysis on Infinite Dimensional Manifolds: The Schrödinger representation in Quantum Field Theory, Brazil Summer School (1989), MIT-CTP/1632.

[54] J. N. Islam, The Schrödinger Equation in Quantum Field Theory, Found. Phys. 24-5 (1994).

[55] J. H. Yee, Schrödinger Picture representation of Quantum Field Theory, SNUTP 92-40, Yonsei University, Seoul, Korea.

[56] K. Symanzik, Nucl. Phys. B 190 (1983) 1; M. Lüscher, Nucl. Phys. B 254 (1985) 52.

[57] M. Lüscher, R. Narayanan, P. Weisz and U. Wolff, The Schrödinger Functional - a Renormalizable Probe for Non-Abelian Gauge Theories, DESY 92-025, CERN-TH. 6410/92.

[58] E. Witten, *Anti de Sitter Space and Holography*, `hep-th/9802150`.

[59] Jae Hyung Yee, `hep-th/9707234`; I. I. Kogan, A. Kovner, Phys. Rev. D51 (1995) 1948.

[60] M. Chaichian and A. Demichev, Path Integrals in Physics, Volume II, Institute of Physics, 2001; M. Masujima, Path Integral Quantization and Stochastic Quantization, Springer, 2000.

[61] M. S. Swanson, Path Integrals and Quantum Processes, Academic Press, 1992.

[62] Ram P. Kanwal, Generalized Functions: Theory and Technique, Birkhäuser, Second Edition, 1997.

[63] Bernard W. Roos, Analytic Functions and Distributions in Physics and Engineering, John Wiley& Sons, 1969.

[64] A. Jaramillo and P. Mansfield, Int. J. Mod. Phys. A 15 (2000) 581; `hep-th/9808067`.

[65] P. Mansfield, Phys. Lett. B 365 (1996) 207.